Inventors (please provide full names):

Earliest Priority Date:

Search Topic:
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

See claims attached. Please do structure search and inventor name(s) search. Display results to show identification of source, and RN##, compound name and structure of identified compounds. Search compounds of Formula III as indicated. See previous searches.

Please call with any questions.

STAFF USE ONLY

Type of Search

Vendors and cost where applicable

Searcher: ______

NA Sequence (#) ______

STN ______

Dialog ______

Searcher Phone #: ______

AA Sequence (#) ______

Questel/Orbit ______

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Structure (#) ______

Medline ______

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Date Searcher Picked Up: ______

Bibliographic ______

In-house sequence systems ______

Date Completed: ______

Litigation ______

Commercial ______ Oligomer ______ Score/Length ______

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Other (specify) ______

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L1   ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:        1999:576785  HCAPLUS  Full-text
DOCUMENT NUMBER:         131:214294
TITLE:                   Preparation of substituted quinazolines and
                         heterocyclic analogs as antagonists or positive
                         modulators of AMPA receptors
INVENTOR(S):             Upasani, Ravi; Cai, Sui X.; Lan, Nancy C.; Wang, Yan;
                         Field, George; Fick, David B.
PATENT ASSIGNEE(S):      Cocensys, Inc., USA
SOURCE:                  PCT Int. Appl., 117 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
LANGUAGE:                English
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
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     WO 9944612           A1    19990910    WO 1999-US4609         19990302
         W:  JP, US
         RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE
     EP 1066039           A1    20010110    EP 1999-911063         19990302
         R:  BE, CH, DE, ES, FR, GB, IT, LI, NL, IE
     JP 2002505288        T     20020219    JP 2000-534214         19990302
     US 6465472           B1    20021015    US 2000-654839         20000901
     US 20030033089       A1    20030213    US 2002-219755         20020816
     US 6765006           B2    20040720
     US 20040162299       A1    20040819    US 2004-772445         20040206 <--
PRIORITY APPLN. INFO.:                       US 1998-76451P      P  19980302
                                             WO 1999-US4609      W  19990302
                                             US 2000-654839      A3 20000901
                                             US 2002-219755      A3 20020816
OTHER SOURCE(S):         MARPAT 131:214294
ED   Entered STN:  14 Sep 1999
GI
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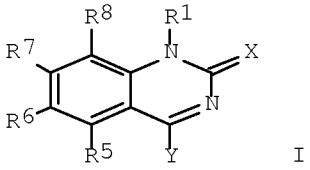

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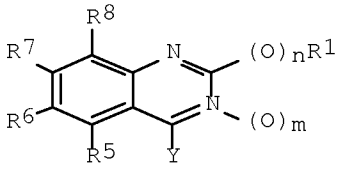

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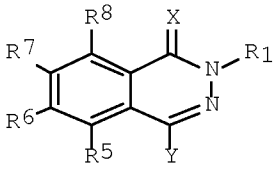

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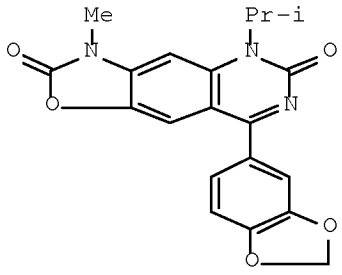

IV

AB Substituted quinazolines and heterocyclic analogs (I, II, and III) [R1 = (un)substituted alkyl, alkenyl, or alkynyl; R5 and R8 = independently H, halogen, NO2, NH2, CN, alkanoylamido, OH, SH, alkoxy, (un)substituted alkyl, (hetero)aryl, heterocyclic, alkenyl, or alkynyl, etc.; R6 and R7 taken together = 5- or 6-membered carbocyclic or heterocyclic ring; X = O or S; Y = (hetero)aryl; n and m = independently 0 or 1] were prepared as antagonists or pos. modulators of AMPA receptors for treatment, prevention, or amelioration of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia. Thus, 3-methyl-5-nitro-2(3H)-benzoxazolone was reduced to the amine over Pt/C in glacial acetic acid. Na cyanoborohydride was added to a suspension of the amine, THF, acetic acid, and acetone followed by treatment with NaOH and water to precipitate 5-(isopropylamino)-3-methyl-2(3H)-benzoxazolone. The substituted amine was converted to the ureido derivative by stirring with KCNO in glacial acetic acid for 5 days. The urea was cyclized with piperonal in benzene and methanesulfonic acid to form the 3,4-dihydrooxazolo[4,5-g]quinazolin-2(1H)-one. The product was reduced by addition of KMnO4 in H2O followed by treatment with formalin to yield 1-isopropyl-4-(3,4-methylenedioxyphenyl)-8-methyl-7-oxooxazolo[4,5-g]quinazolin-2(1H)-one (IV). Selected compds. of the invention were tested for preferred binding to AMPA receptors and exhibited IC50 values ranging from 0.2 to 13 μM. The anticonvulsant activity of the AMPA antagonists was evaluated in the Maximal Electroshock-induced Seizure (MES) test. MES ED50 values ranged from 1 to 10 mg/kg i.v.

IC ICM A61K031-50
ICS A61K031-505; C07D237-26; C07D239-70; C07D491-04; C07D491-048; C07D491-056; C07D498-04

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

ST quinazoline AMPA receptor antagonist pos modulator prepn; ischemia amyotrophic lateral sclerosis schizophrenia treatment quinazoline prepn; anticonvulsant quinazoline prepn; analgesic quinazoline prepn; excitatory amino acid neurotransmitter antagonist quinazoline prepn; learning cognition enhancer quinazoline prepn

IT Glutamate receptors
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(AMPA-binding, agonists; preparation of substituted quinazolines and

heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

IT Nervous system
(amyotrophic lateral sclerosis, treatment; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

IT Nerve
Nervous system
(degeneration, treatment; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

IT Neurotransmitter antagonists
(excitatory amino acid; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

IT Heart, disease
(ischemia, treatment; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

IT Cytoprotective agents
(neuroprotectants; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

IT Analgesics
Anti-ischemic agents
Anticonvulsants
Cognition enhancers
Glutamate agonists
(preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

IT Schizophrenia
(treatment; preparation of substituted quinazolines and heterocyclic analogs
as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

IT 85575-56-0P 99584-09-5P 243134-92-1P 243134-93-2P 243134-94-3P
243134-95-4P 243134-96-5P 243134-97-6P 243134-98-7P 243134-99-8P
243135-00-4P 243135-01-5P 243135-02-6P 243135-03-7P 243135-04-8P
243135-05-9P 243135-06-0P 243135-07-1P 243135-08-2P 243135-09-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

IT 243135-42-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of substituted quinazolines and heterocyclic analogs as

antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

IT 243135-18-4 243135-19-5 243135-20-8 243135-21-9 243135-22-0
243135-23-1 243135-24-2 243135-25-3 243135-26-4 243135-27-5
243135-28-6 243135-29-7 243135-30-0 243135-31-1 243135-32-2
243135-33-3 243135-34-4 243135-35-5 243135-36-6 243135-37-7
243135-38-8 243135-39-9 243135-40-2 243135-41-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

IT 60-56-0, 2-Mercapto-1-methylimidazole 66-99-9, 2-Naphthaldehyde
67-64-1, 2-Propanone, reactions 75-30-9, 2-Iodopropane 92-54-6
100-10-7, 4-(Dimethylamino)benzaldehyde 100-39-0, Benzyl bromide
100-52-7, Benzaldehyde, reactions 110-85-0, Piperazine, reactions
115-80-0, Triethyl orthopropionate 120-57-0, Piperonal 123-75-1,
Pyrrolidine, reactions 288-32-4, Imidazole, reactions 500-22-1,
3-Pyridinecarboxaldehyde 656-42-8 1544-85-0,
5-Amino-2,2-difluoro-1,3-benzodioxole 3218-36-8, 4-Phenylbenzaldehyde
3889-13-2 4584-46-7, 2-(Dimethylamino)ethyl chloride hydrochloride
7051-34-5, (Bromomethyl)cyclopropane 13669-42-6,
3-Quinolinecarboxaldehyde 14268-66-7, 3,4-(Methylenedioxy)aniline
15952-61-1, 6-Chloropiperonal 16081-45-1, 5-Amino-1,4-benzodioxane
22013-33-8, 1,4-Benzodioxan-6-amine 24425-40-9 25054-53-9,
Piperonyloyl chloride 29668-44-8, 1,4-Benzodioxan-6-carboxaldehyde
30084-91-4, 5-Indancarboxaldehyde 32953-14-3,
N-Ethyl-3,4-(methylenedioxy)aniline 94614-83-2 101084-60-0
109258-03-9 243135-10-6 243135-11-7 243135-12-8 243135-13-9
243135-14-0 243135-15-1 243135-16-2 243135-17-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

IT 10368-14-6P 33095-75-9P 33095-79-3P 33095-82-8P 33095-94-2P
34060-22-5P 40484-04-6P 59856-06-3P 63546-19-0P 85575-57-1P
164526-15-2P 243133-76-8P 243133-77-9P 243133-78-0P 243133-79-1P
243133-81-5P 243133-82-6P 243133-85-9P 243133-86-0P 243133-88-2P
243133-90-6P 243133-92-8P 243133-94-0P 243133-95-1P 243133-96-2P
243133-97-3P 243133-98-4P 243133-99-5P 243134-07-8P 243134-13-6P
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243134-66-9P 243134-73-8P
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(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

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243134-77-2P 243134-78-3P 243134-79-4P 243134-80-7P 243134-81-8P
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L2 ANSWER 1 OF 1 WPIX COPYRIGHT 2008 THOMSON REUTERS on STN
ACCESSION NUMBER: 1999-540736 [45] WPIX
DOC. NO. CPI: C1999-157966 [45]
TITLE: Substituted quinazolines and pharmaceutically acceptable salts and prodrugs as alpha-amino-3-hydroxy-5-methylisozazole-4-propionic acid receptor modulators - used to treat neuronal loss associated with stroke and neurodegenerative diseases
DERWENT CLASS: B02
INVENTOR: CAI S X; FICK D B; FIELD G; LAN N C; UPASANI R; WANG Y
PATENT ASSIGNEE: (COCE-N) COCENSYS INC; (EURO-N) EUROCELTIQUE SA
COUNTRY COUNT: 21

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 9944612	A1	19990910	(199945)*	EN	117[0]	
EP 1066039	A1	20010110	(200103)	EN		
JP 2002505288	W	20020219	(200216)	JA	142	
US 6465472	B1	20021015	(200271)	EN		
US 20030033089	A1	20030213	(200314)	EN		
US 6765006	B2	20040720	(200448)	EN		
US 20040162299	A1	20040819	(200455)	EN		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 9944612 A1		WO 1999-US4609	19990302
US 6465472 B1	Provisional	US 1998-76451P	19980302
US 20030033089 A1	Provisional	US 1998-76451P	19980302
US 6765006 B2	Provisional	US 1998-76451P	19980302
US 20040162299 A1	Provisional	US 1998-76451P	19980302
EP 1066039 A1		EP 1999-911063	19990302
EP 1066039 A1		WO 1999-US4609	19990302
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US 6765006 B2	Cont of	WO 1999-US4609	19990302
US 20040162299 A1	Cont of	WO 1999-US4609	19990302
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US 20030033089 A1	Div Ex	US 2000-654839	20000901
US 20040162299 A1	Div Ex	US 2000-654839	20000901
US 6765006 B2	Div Ex	US 2001-654839	20010901
US 20030033089 A1		US 2002-219755	20020816
US 6765006 B2		US 2002-219755	20020816
US 20040162299 A1	Div Ex	US 2002-219755	20020816
US 20040162299 A1		US 2004-772445	20040206

FILING DETAILS:

PATENT NO	KIND		PATENT NO	
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US 6765006	B2	Div ex	US 6465472	B
US 20040162299	A1	Div ex	US 6465472	B
EP 1066039	A1	Based on	WO 9944612	A
JP 2002505288	W	Based on	WO 9944612	A

PRIORITY APPLN. INFO: US 1998-76451P 19980302
WO 1999-US4609 19990302
US 2000-654839 19990901
US 2001-654839 20010901
US 2002-219755 20020816
US 2004-772445 20040206

INT. PATENT CLASSIF.:
MAIN: C07D491-056
INDEX: C07D239:80; C07D317:10

IPC RECLASSIF.: A61K0031-502 [I,A]; A61K0031-502 [I,C]; A61K0031-5025 [I,A]; A61K0031-5025 [I,C]; A61K0031-517 [I,A]; A61K0031-517 [I,C]; A61K0031-519 [I,A]; A61K0031-519 [I,C]; A61P0025-00 [I,C]; A61P0025-08 [I,A]; A61P0025-16 [I,A]; A61P0025-18 [I,A]; A61P0025-28 [I,A]; A61P0009-00 [I,C]; A61P0009-10 [I,A]; C07D0237-00 [I,C]; C07D0237-32 [I,A]; C07D0239-00 [I,C]; C07D0239-82 [I,A]; C07D0405-00 [I,C]; C07D0405-04 [I,A]; C07D0491-00 [I,C]; C07D0491-04 [I,A]; C07D0491-048 [I,A]; C07D0491-056 [I,A]; C07D0498-00 [I,C]; C07D0498-04 [I,A]; C07D0521-00 [I,A]; C07D0521-00 [I,C]

ECLA: C07D0239-82; C07D0491-04+317A+237A; C07D0491-04+317A+239A; C07D0491-04+319A+239A; C07D0498-04+263A+239A; C07D0521-00B1C8

ICO: M07D0239:82

USCLASS NCLM: 514/232.800

NCLS: 514/266.310; 514/267.000; 544/115.000; 544/250.000; 544/284.000; 544/286.000

BASIC ABSTRACT:

WO 1999044612 A1 UPAB: 20060503

NOVELTY - Substituted quinazolines and their pharmaceutically acceptable salts and prodrugs.

DETAILED DESCRIPTION - Substituted quinazolines are of formula (I):

R1 = alkyl, haloalkyl, aminoalkyl, alkenyl, alkynyl, aralkyl, aralkenyl, aralkynyl, heteroaralkyl, carbocycloalkyl, heterocycloalkyl, hydroxyalkyl, cyanoalkyl, alkanoylamidoalkyl, alkanoyloxyalkyl, azidoalkyl, alkenyloxyalkyl or alkoxyalkyl;

R6, R7 taken together = 5-6-membered carbocyclic or heterocyclic ring;

R5, R8 = H, halo, haloalkyl, aryl, heterocycle, heteroaryl, alkyl, alkenyl, alkynyl, aralkyl, aralkenyl, aralkynyl, hydroxyalkyl, nitro, amino, cyano, alkanoylamido, hydroxy, thiol, alkanoyloxy, alkoxy, carboxy, carbonylamido or thioalkoxy;

X = O or S; and

Y = aryl or heteroaryl.

INDEPENDENT CLAIMS are also included for:

(1) compounds of formula (II);

(2) compounds of formula (III)

n, z = 0-1.

ACTIVITY - Neuroprotective; neuroregenerative; anxiolytic; anti-psychotic; anticonvulsant; analgesic; anti-migraine; anti-glaucoma; anti-retinitis; anti-urinary incontinence; anesthetic; cognitive improving; anti-schizophrenia; anti-myoclonus.

MECHANISM OF ACTION - Alpha-amino-3-hydroxy-5-methylisozazole-4-propionic acid (AMPA) ionotropic receptor antagonists; AMPA positive modulators.

USE - Used to treat, prevent or ameliorate neuronal loss associated with stroke, ischemia including global ischemia especially as a result of cardiac arrest, CNS trauma, hypoglycemia or surgery, to treat or ameliorate neurodegenerative diseases including Alzheimer's disease, amyotrophic lateral sclerosis, Huntington's disease, Parkinson's disease and Down's syndrome, to treat, prevent or ameliorate adverse consequences of the overstimulation of excitatory amino acids, to treat, prevent or ameliorate anxiety, psychosis, convulsions, chronic pain, migraine headache, glaucoma, retinitis and urinary incontinence, to induce anesthesia, to enhance learning and cognition, to treat or ameliorate schizophrenia or myoclonus (claimed). Also used to treat acute neurological disorders such as domoic acid poisoning, cerebral ischemia, stroke, spinal cord trauma, hypoxia, anoxia, carbon monoxide, cyanide or manganese poisoning, hypoglycemia, mechanical trauma to the nervous system, neuronal injury associated with HIV and AIDS, AIDS dementia, neuropathic pain syndrome, olivopontocerebral atrophy, mitochondrial abnormalities, hepatic encephalopathy, Tourette's syndrome, drug addiction, acute and chronic pain, pain associated with post-therapeutic neuralgia, interstitial cystitis, osteoarthritis, spinal cord injury, diabetic neuropathy, generalized anxiety disorder, phobic disorders, obsessive-compulsvie disorders, panic disorders and post-traumatic stress disorder.

MANUAL CODE: CPI: B06-E05; B14-C01; B14-C09A; B14-F01; B14-F01B; B14-F02D1; B14-J01A3; B14-J01A4; B14-J01B3; B14-J01B4; B14-J07; B14-M01C; B14-N03; B14-N07D; B14-N16; B14-S01

AN 1999-540736 [45] WPIX

DC B02

IC ICM C07D491-056

ICI C07D239:80; C07D317:10

IPCR A61K0031-502 [I,A]; A61K0031-502 [I,C]; A61K0031-5025 [I,A]; A61K0031-5025 [I,C]; A61K0031-517 [I,A]; A61K0031-517 [I,C]; A61K0031-519 [I,A]; A61K0031-519 [I,C]; A61P0025-00 [I,C]; A61P0025-08 [I,A]; A61P0025-16 [I,A]; A61P0025-18 [I,A]; A61P0025-28 [I,A]; A61P0009-00 [I,C]; A61P0009-10 [I,A]; C07D0237-00 [I,C]; C07D0237-32 [I,A]; C07D0239-00

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     C07D0491-00 [I,C]; C07D0491-04 [I,A]; C07D0491-048 [I,A]; C07D0491-056
     [I,A]; C07D0498-00 [I,C]; C07D0498-04 [I,A]; C07D0521-00 [I,A];
     C07D0521-00 [I,C]
EPC  C07D0239-82; C07D0491-04+317A+237A; C07D0491-04+317A+239A;
     C07D0491-04+319A+239A; C07D0498-04+263A+239A; C07D0521-00B1C8
ICO  M07D0239:82
NCL  NCLM  514/232.800
     NCLS  514/266.310; 514/267.000; 544/115.000; 544/250.000; 544/284.000;
           544/286.000
IT   UPIT 20060503
     232212-CL 232212-NEW; 232213-CL 232213-NEW; 232214-CL 232214-NEW;
     232215-CL 232215-NEW; 232216-CL 232216-NEW; 232217-CL 232217-NEW;
     232218-CL 232218-NEW; 232219-CL 232219-NEW; 232220-CL 232220-NEW;
     232874-CL 232874-NEW; 232875-CL 232875-NEW; 232876-CL 232876-NEW;
     232877-CL 232877-NEW; 232878-CL 232878-NEW; 232879-CL 232879-NEW;
     232880-CL 232880-NEW; 232881-CL 232881-NEW; 0006-89701-CL 0006-89701-NEW;
     0006-89702-CL 0006-89702-NEW; 0006-89703-CL 0006-89703-NEW
MC   CPI: B06-E05; B14-C01; B14-C09A; B14-F01; B14-F01B; B14-F02D1; B14-J01A3;
           B14-J01A4; B14-J01B3; B14-J01B4; B14-J07; B14-M01C; B14-N03;
           B14-N07D; B14-N16; B14-S01
CMC  UPB   20060503
     M2 *01*   D014 E530 G021 G221 H2 H211 J5 J521 L9 L921 M1 M115 M210 M212
               M273 M281 M320 M412 M511 M520 M531 M540 M710 P411 P412 P421 P440
               P442 P446 P522 P625 P646  M905 M904
               RIN: 02803
               DCN: RA0O40-N RA0O40-T
               DCR: 232212-N 232212-T
     M2 *02*   J5 J521 L9 L921 M1 M115 M210 M213 M232 M273 M281 M320 M412 M511
               M520 M531 M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646
               M905 M904
               RIN: 02803
               DCN: RA0O41-N RA0O41-T
               DCR: 232213-N 232213-T
     M2 *03*   D014 D022 D140 E530 G030 G530 H2 H211 J5 J521 L9 L921 M1 M115
               M280 M311 M321 M342 M373 M391 M412 M512 M520 M710 P411 P412 P421
               P440 P442 P446 P522 P625 P646  M905
               RIN: 02803
               DCN: RA0O42-N RA0O42-T
               DCR: 232214-N 232214-T
     M2 *04*   D014 D022 D140 E530 H1 H103 H181 H2 H211 J5 J521 L9 L921 M1 M115
               M210 M212 M273 M282 M312 M321 M332 M342 M383 M391 M412 M512 M520
               M530 M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646
               M905 M904
               RIN: 02803
               DCN: RA0O43-N RA0O43-T
               DCR: 232215-N 232215-T
     M2 *05*   D014 D022 D140 E530 H2 H211 H7 H731 J5 J521 L9 L921 M1 M115 M210
               M213 M231 M273 M281 M320 M412 M512 M520 M530 M540 M710 P411 P412
               P421 P440 P442 P446 P522 P625 P646  M905 M904
               RIN: 02803
               DCN: RA0O44-N RA0O44-T
               DCR: 232216-N 232216-T
     M2 *06*   D013 D022 D140 E530 H1 H103 H181 H5 H521 H8 L921 M1 M115 M210
               M212 M273 M282 M312 M321 M332 M342 M383 M391 M412 M512 M520 M530
               M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646  M905
               M904
               RIN: 02803
               DCN: RA0O45-N RA0O45-T
               DCR: 232217-N 232217-T
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M2 *07*   D013 D022 D140 E530 H1 H103 H181 H5 H521 H8 L921 M1 M115 M210
          M211 M273 M282 M312 M321 M332 M342 M383 M391 M412 M512 M520 M530
          M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646  M905
          M904
          RIN: 02803
          DCN: RA0O46-N RA0O46-T
          DCR: 232218-N 232218-T
M2 *08*   D013 D022 D140 E530 H1 H100 H181 H5 H521 H8 L921 M1 M115 M280
          M312 M321 M332 M342 M383 M391 M412 M512 M520 M530 M540 M710 P411
          P412 P421 P440 P442 P446 P522 P625 P646  M905 M904
          RIN: 02803
          DCN: RA0O47-N RA0O47-T
          DCR: 232219-N 232219-T
M2 *09*   D013 D022 D140 E530 F011 F423 H1 H181 H2 H201 H5 H521 H8 L921 M1
          M115 M280 M312 M321 M332 M342 M383 M391 M412 M512 M521 M530 M540
          M710 P411 P412 P421 P440 P442 P446 P522 P625 P646  M905 M904
          RIN: 02803
          DCN: RA0O48-N RA0O48-T
          DCR: 232220-N 232220-T
M2 *10*   D014 D022 D140 E530 H2 H211 J0 J011 J2 J271 J5 J521 L9 L941 M1
          M115 M210 M212 M272 M281 M312 M321 M332 M342 M381 M391 M412 M512
          M520 M530 M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646
          M905 M904
          RIN: 02805
          DCN: RA0ON1-N RA0ON1-T
          DCR: 232874-N 232874-T
M2 *11*   D014 D022 D140 E530 F011 F423 H1 H181 H2 H201 H211 J5 J521 L9
          L941 M1 M115 M280 M312 M321 M332 M342 M383 M391 M412 M512 M521
          M530 M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646
          M905 M904
          RIN: 02805
          DCN: RA0ON2-N RA0ON2-T
          DCR: 232875-N 232875-T
M2 *12*   D014 D022 D140 E530 F011 F433 H1 H181 H2 H201 H211 J5 J521 L9
          L941 M1 M115 M280 M312 M321 M332 M342 M383 M391 M412 M512 M521
          M530 M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646
          M905 M904
          RIN: 02805
          DCN: RA0ON3-N RA0ON3-T
          DCR: 232876-N 232876-T
M2 *13*   D013 D022 D140 E530 J5 J521 L9 L941 M1 M115 M280 M320 M412 M512
          M520 M530 M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646
          M905 M904
          RIN: 02805
          DCN: RA0ON4-N RA0ON4-T
          DCR: 232877-N 232877-T
M2 *14*   D014 D022 D140 E530 F011 F521 H1 H181 H2 H201 H211 J5 J521 L9
          L941 M1 M115 M280 M312 M321 M332 M342 M383 M391 M412 M512 M521
          M530 M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646
          M905 M904
          RIN: 02805
          DCN: RA0ON5-N RA0ON5-T
          DCR: 232878-N 232878-T
M2 *15*   D014 D022 D140 E530 H2 H211 J5 J521 L9 L941 M1 M115 M210 M212
          M273 M281 M320 M412 M512 M520 M530 M540 M710 P411 P412 P421 P440
          P442 P446 P522 P625 P646  M905 M904
          RIN: 02805
          DCN: RA0ON6-N RA0ON6-T
          DCR: 232879-N 232879-T
M2 *16*   M1 M115 M210 M211 M273 M282 M312 M321 M332 M342 M383 M391 M412
```

M512 M520 M530 M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646 M905 M904
RIN: 02805
DCN: RA0ON7-N RA0ON7-T
DCR: 232880-N 232880-T

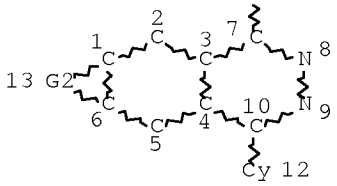
M2 *17* D014 D022 D140 E530 H1 H103 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646 M905
RIN: 02805
DCN: RA0ON8-N RA0ON8-T
DCR: 232881-N 232881-T

M2 *18* D014 D021 D023 D040 F010 F019 F020 F021 F029 G010 G019 G020 G021 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H141 H142 H181 H2 H211 H341 H342 H401 H402 H403 H441 H442 H481 H482 H483 H494 H498 H541 H542 H600 H608 H609 H641 H642 H681 H682 H683 H689 H713 H715 H716 H721 H722 H723 H731 J011 J012 J013 J131 J132 J241 J242 J341 J342 J371 J5 J521 J592 L143 L145 L199 L640 L650 L699 L9 L921 L922 M1 M112 M113 M114 M115 M116 M119 M122 M124 M129 M132 M135 M139 M150 M210 M211 M212 M213 M214 M215 M216 M220 M221 M222 M223 M224 M225 M226 M231 M232 M233 M240 M262 M272 M273 M280 M281 M282 M283 M311 M312 M313 M314 M315 M316 M320 M321 M322 M323 M331 M332 M333 M334 M340 M342 M343 M344 M349 M353 M362 M373 M381 M383 M391 M392 M393 M412 M511 M520 M521 M522 M523 M530 M531 M532 M533 M540 M541 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646 M905 M904
MCN: 0006-89701-N 0006-89701-T

M2 *19* D014 D021 D023 D040 F010 F019 F020 F021 F029 G010 G019 G020 G021 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H141 H142 H181 H2 H211 H341 H342 H401 H402 H403 H441 H442 H481 H482 H483 H494 H498 H541 H542 H600 H608 H609 H641 H642 H681 H682 H683 H689 H713 H715 H716 H721 H722 H723 H731 J011 J012 J013 J131 J132 J241 J242 J341 J342 J371 J5 J521 J592 L143 L145 L199 L640 L650 L699 L9 L941 L943 M1 M112 M113 M114 M115 M116 M119 M122 M124 M129 M132 M135 M139 M150 M210 M211 M212 M213 M214 M215 M216 M220 M221 M222 M223 M224 M225 M226 M231 M232 M233 M240 M262 M272 M273 M280 M281 M282 M283 M311 M312 M313 M314 M315 M316 M320 M321 M322 M323 M331 M332 M333 M334 M340 M342 M343 M344 M349 M353 M362 M373 M381 M383 M391 M392 M393 M412 M511 M520 M521 M522 M523 M530 M531 M532 M533 M540 M541 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646 M905 M904
MCN: 0006-89702-N 0006-89702-T

M2 *20* D013 D014 D021 D023 D040 F010 F019 F020 F021 F029 G010 G019 G020 G021 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H141 H142 H181 H341 H342 H401 H402 H403 H441 H442 H481 H482 H483 H494 H498 H521 H541 H542 H600 H608 H609 H641 H642 H681 H682 H683 H689 H715 H721 H722 H723 H731 J011 J012 J013 J131 J132 J241 J242 J341 J342 J371 K850 L143 L145 L199 L640 L650 L660 L699 L921 M1 M112 M113 M114 M115 M116 M119 M122 M123 M124 M125 M126 M129 M132 M135 M139 M141 M150 M210 M211 M212 M213 M214 M215 M216 M220 M221 M222 M223 M224 M225 M226 M231 M232 M233 M240 M262 M272 M280 M281 M282 M283 M311 M312 M313 M314 M315 M316 M320 M321 M322 M323 M331 M332 M333 M334 M340 M342 M343 M344 M349 M353 M362 M372 M373 M381 M383 M391 M392 M393 M412 M511 M520 M521 M522 M523 M530 M531 M532 M533 M540 M541 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646 M905 M904
MCN: 0006-89703-N 0006-89703-T

```
=> => d que stat l10
L8               STR
```



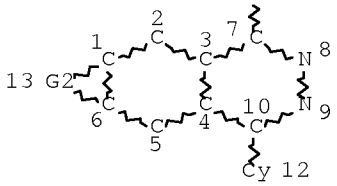

```
VAR G1=14/15
REP G2=(1-6) A
NODE ATTRIBUTES:
CONNECT IS E1  RC AT  14
CONNECT IS E1  RC AT  15
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT  12
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  15

STEREO ATTRIBUTES: NONE
L10          56 SEA FILE=REGISTRY SSS FUL L8

100.0% PROCESSED   83282 ITERATIONS                                56 ANSWERS
SEARCH TIME: 00.00.04


=> d que stat l15
L8               STR
```

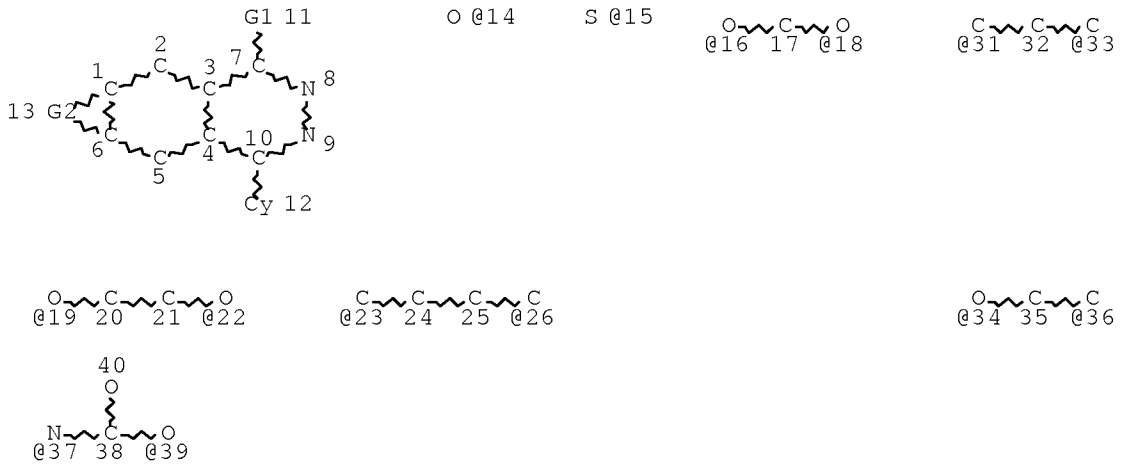



```
VAR G1=14/15
REP G2=(1-6) A
NODE ATTRIBUTES:
CONNECT IS E1  RC AT  14
CONNECT IS E1  RC AT  15
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT  12
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
```

NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
L10 56 SEA FILE=REGISTRY SSS FUL L8
L13 STR



VAR G1=14/15
VAR G2=16-6 18-1/19-6 22-1/31-6 33-1/23-6 26-1/34-6 36-1/36-6 34-1/37-6 3
9-1/39-6 37-1
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 14
CONNECT IS E1 RC AT 15
CONNECT IS E1 RC AT 40
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 12
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 36

STEREO ATTRIBUTES: NONE
L15 37 SEA FILE=REGISTRY SUB=L10 SSS FUL L13

100.0% PROCESSED 56 ITERATIONS 37 ANSWERS
SEARCH TIME: 00.00.01

=> d que nos l17
L8 STR
L10 56 SEA FILE=REGISTRY SSS FUL L8
L13 STR
L15 37 SEA FILE=REGISTRY SUB=L10 SSS FUL L13
L17 ANALYZE PLU=ON L15 1- LC : 8 TERMS

=> d l17 1-
L17 ANALYZE L15 1- LC : 8 TERMS

TERM # # OCC # DOC % DOC LC

```
------ ------- ------ ------ ---------------
     1      36     36  97.30 CA
     2      36     36  97.30 CAPLUS
     3      21     21  56.76 CASREACT
     4      14     14  37.84 TOXCENTER
     5       7      7  18.92 USPATFULL
     6       1      1   2.70 BEILSTEIN
     7       1      1   2.70 CAOLD
     8       1      1   2.70 CHEMCATS
*********  END OF L17***


=> d que nos l31
L1             1 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  US2004-772445/APPS
L8               STR
L10           56 SEA FILE=REGISTRY SSS FUL L8
L13              STR
L15           37 SEA FILE=REGISTRY SUB=L10 SSS FUL L13
L19              QUE  SPE=ON  ABB=ON  PLU=ON  UPASANI, R?/AU
L20              QUE  SPE=ON  ABB=ON  PLU=ON  CAI, S?/AU
L21              QUE  SPE=ON  ABB=ON  PLU=ON  LAN, N?/AU
L22              QUE  SPE=ON  ABB=ON  PLU=ON  WANG, Y?/AU
L23              QUE  SPE=ON  ABB=ON  PLU=ON  FIELD, G?/AU
L24              QUE  SPE=ON  ABB=ON  PLU=ON  FICK, D?/AU
L25              QUE  SPE=ON  ABB=ON  PLU=ON  (COCENSYS OR (PURDUE(1W)PHAR
                 MA) OR (EURO(1W)CELTIQUE))/CS,SO,PA
L27           17 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L15
L28            1 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L27 AND (L19 OR L20
                 OR L21 OR L22 OR L23 OR L24 OR L25)
L29            1 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L1 AND L28
L30            1 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  (L28 OR L29)
L31           16 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L27 NOT L30


=> d his l34

     (FILE 'USPATFULL, USPATOLD, USPAT2, CASREACT, TOXCENTER' ENTERED AT
     15:31:58 ON 04 DEC 2008)
L34            6 S L32 NOT L33

=> d que nos l34
L8               STR
L10           56 SEA FILE=REGISTRY SSS FUL L8
L13              STR
L15           37 SEA FILE=REGISTRY SUB=L10 SSS FUL L13
L19              QUE  SPE=ON  ABB=ON  PLU=ON  UPASANI, R?/AU
L20              QUE  SPE=ON  ABB=ON  PLU=ON  CAI, S?/AU
L21              QUE  SPE=ON  ABB=ON  PLU=ON  LAN, N?/AU
L22              QUE  SPE=ON  ABB=ON  PLU=ON  WANG, Y?/AU
L23              QUE  SPE=ON  ABB=ON  PLU=ON  FIELD, G?/AU
L24              QUE  SPE=ON  ABB=ON  PLU=ON  FICK, D?/AU
L25              QUE  SPE=ON  ABB=ON  PLU=ON  (COCENSYS OR (PURDUE(1W)PHAR
                 MA) OR (EURO(1W)CELTIQUE))/CS,SO,PA
L32            9 SEA L15
L33            3 SEA L32 AND (L19 OR L20 OR L21 OR L22 OR L23 OR L24 OR L25)
L34            6 SEA L32 NOT L33

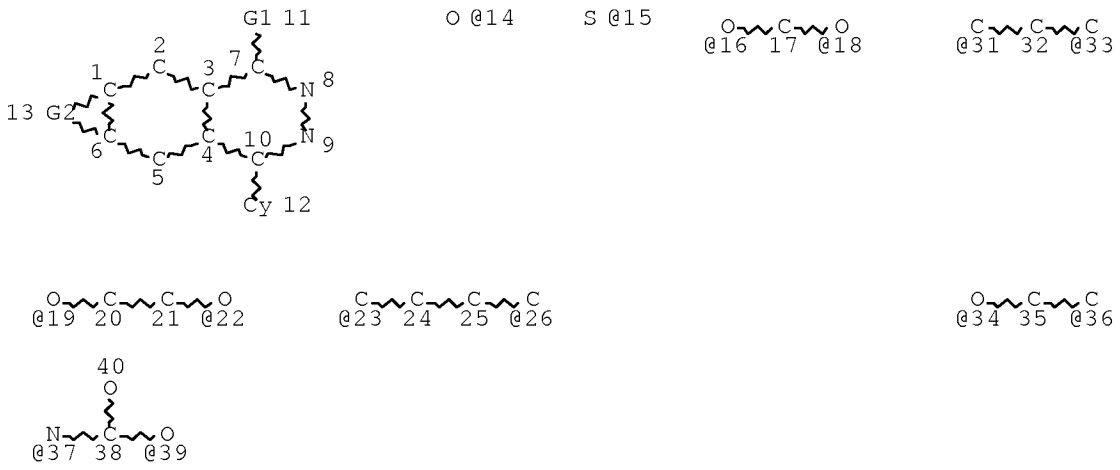

=> d que nos l35
L8               STR
```

```
L10           56 SEA FILE=REGISTRY SSS FUL L8
L13              STR
L15           37 SEA FILE=REGISTRY SUB=L10 SSS FUL L13
L35            1 SEA FILE=CAOLD SPE=ON  ABB=ON  PLU=ON  L15


=> d que nos l36
L36            2 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  CA52:15486I/OREF


=> d que nos l37
L8               STR
L10           56 SEA FILE=REGISTRY SSS FUL L8
L13              STR
L15           37 SEA FILE=REGISTRY SUB=L10 SSS FUL L13
L37            3 SEA FILE=CHEMCATS SPE=ON  ABB=ON  PLU=ON  L15


=> d que stat l41
L13              STR
```




```
VAR G1=14/15
VAR G2=16-6 18-1/19-6 22-1/31-6 33-1/23-6 26-1/34-6 36-1/36-6 34-1/37-6 3
9-1/39-6 37-1
NODE ATTRIBUTES:
CONNECT IS E1  RC AT  14
CONNECT IS E1  RC AT  15
CONNECT IS E1  RC AT  40
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT  12
DEFAULT ECLEVEL IS LIMITED

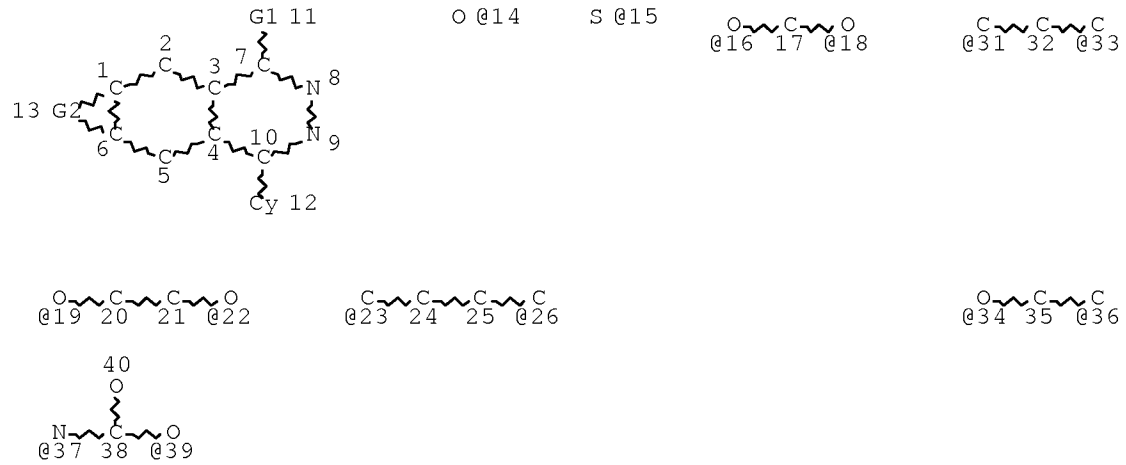
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  36

STEREO ATTRIBUTES: NONE
L41            4 SEA FILE=CHEMINFORMRX SSS FUL L13 (     8 REACTIONS)

100.0% DONE    1376 VERIFIED       8 HIT RXNS                      4 DOCS
SEARCH TIME: 00.00.22
```

```
=> d que nos l43
L13             STR
L19             QUE  SPE=ON  ABB=ON  PLU=ON  UPASANI, R?/AU
L20             QUE  SPE=ON  ABB=ON  PLU=ON  CAI, S?/AU
L21             QUE  SPE=ON  ABB=ON  PLU=ON  LAN, N?/AU
L22             QUE  SPE=ON  ABB=ON  PLU=ON  WANG, Y?/AU
L23             QUE  SPE=ON  ABB=ON  PLU=ON  FIELD, G?/AU
L24             QUE  SPE=ON  ABB=ON  PLU=ON  FICK, D?/AU
L25             QUE  SPE=ON  ABB=ON  PLU=ON  (COCENSYS OR (PURDUE(1W)PHAR
                MA) OR (EURO(1W)CELTIQUE))/CS,SO,PA
L41           4 SEA FILE=CHEMINFORMRX SSS FUL L13 (     8 REACTIONS)
L42           0 SEA FILE=CHEMINFORMRX SPE=ON  ABB=ON  PLU=ON  L41 AND (L19 OR
                L20 OR L21 OR L22 OR L23 OR L24 OR L25)
L43           4 SEA FILE=CHEMINFORMRX SPE=ON  ABB=ON  PLU=ON  L41 NOT L42


=> d que stat l45
L13             STR
```




```
VAR G1=14/15
VAR G2=16-6 18-1/19-6 22-1/31-6 33-1/23-6 26-1/34-6 36-1/36-6 34-1/37-6 3
9-1/39-6 37-1
NODE ATTRIBUTES:
CONNECT IS E1  RC AT  14
CONNECT IS E1  RC AT  15
CONNECT IS E1  RC AT  40
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT  12
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  36

STEREO ATTRIBUTES: NONE
L45           8 SEA FILE=WPIX SSS FUL L13

100.0% PROCESSED     599 ITERATIONS                          8 ANSWERS
```

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SEARCH TIME: 00.00.04


=> d que nos l51
L2             1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  US2004-772445/APPS
L13              STR
L19              QUE  SPE=ON  ABB=ON  PLU=ON  UPASANI, R?/AU
L20              QUE  SPE=ON  ABB=ON  PLU=ON  CAI, S?/AU
L21              QUE  SPE=ON  ABB=ON  PLU=ON  LAN, N?/AU
L22              QUE  SPE=ON  ABB=ON  PLU=ON  WANG, Y?/AU
L23              QUE  SPE=ON  ABB=ON  PLU=ON  FIELD, G?/AU
L24              QUE  SPE=ON  ABB=ON  PLU=ON  FICK, D?/AU
L25              QUE  SPE=ON  ABB=ON  PLU=ON  (COCENSYS OR (PURDUE(1W)PHAR
                 MA) OR (EURO(1W)CELTIQUE))/CS,SO,PA
L45            8 SEA FILE=WPIX SSS FUL L13
L46            1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  (RA0ON1/DCN OR RA0ON2/DCN
                  OR RA0ON3/DCN OR RA0ON4/DCN OR RA0ON5/DCN OR RA0ON6/DCN OR
                 RA0ON7/DCN OR RA0ON8/DCN) OR L45/DCR
L47            1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L46 AND (L19 OR L20 OR
                 L21 OR L22 OR L23 OR L24 OR L25)
L49            1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L47 AND L2
L50            1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L47 OR L49
L51            0 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L46 NOT L50


=> dup rem l31 l34 l35 l36 l37 l43 l51
L51 HAS NO ANSWERS
DUPLICATE IS NOT AVAILABLE IN 'CAOLD, CHEMCATS, CHEMINFORMRX'.
ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE
FILE 'HCAPLUS' ENTERED AT 15:45:19 ON 04 DEC 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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PROCESSING COMPLETED FOR L31
PROCESSING COMPLETED FOR L34
PROCESSING COMPLETED FOR L35
PROCESSING COMPLETED FOR L36
PROCESSING COMPLETED FOR L37
PROCESSING COMPLETED FOR L43
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PROCESSING COMPLETED FOR L51
L55          24 DUP REM L31 L34 L35 L36 L37 L43 L51 (8 DUPLICATES REMOVED)
                ANSWERS '1-16' FROM FILE HCAPLUS
                ANSWER '17' FROM FILE CAOLD
                ANSWERS '18-20' FROM FILE CHEMCATS
                ANSWERS '21-24' FROM FILE CHEMINFORMRX


=> file stnguide
FILE 'STNGUIDE' ENTERED AT 15:45:37 ON 04 DEC 2008
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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov 21, 2008 (20081121/UP).
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=> d ibib ed abs hitind hitstr 1-16
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CAOLD, CHEMCATS, CHEMINFORMRX' -
CONTINUE? (Y)/N:y



L55  ANSWER 1 OF 24  HCAPLUS  COPYRIGHT 2008 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         2007:1295143  HCAPLUS  Full-text
DOCUMENT NUMBER:          148:168645
TITLE:                    Iptycene-Derived Pyridazines and Phthalazines
AUTHOR(S):                Bouffard, Jean; Eaton, Robert F.; Mueller, Peter;
                          Swager, Timothy M.
CORPORATE SOURCE:         Department of Chemistry, Massachusetts Institute of
                          Technology, Cambridge, MA, 02139, USA
SOURCE:                   Journal of Organic Chemistry (2007), 72(26),
                          10166-10180
                          CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER:                American Chemical Society
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
OTHER SOURCE(S):          CASREACT 148:168645
ED   Entered STN:  15 Nov 2007
AB    The synthesis of new heterocyclic oligo(phenylene) analogs based on soluble,
      non-aggregating 1,2-diazines is reported.  Improved palladium-catalyzed
      reductive coupling methods were developed to allow for the preparation of
      large quantities of iptycene-derived bipyridazine compds. and biphthalazine
      compds., and the controlled synthesis of well-defined oligomers up to
      sexipyridazine.  Crystallog., spectroscopic, and computational evidence
      indicate that in these analogs, hindrance at the ortho position is relaxed
      relative to poly(phenylenes).  The resulting building blocks are promising for
      incorporation in conjugated electronics materials and as new iptycene-derived
      ligands for transition metals.
CC   28-15 (Heterocyclic Compounds (More Than One Hetero Atom))
IT   1625-81-6P   1625-82-7P   1625-83-8P,
     9,10-Dihydro-9,10(3',4')-furanoanthracene-12,14-dione   56306-24-2P
     56306-43-5P   123685-23-4P   272111-33-8P   937081-42-0P   937081-43-1P
     937081-49-7P   937081-50-0P   1001639-33-3P   1001639-35-5P
     1001639-36-6P   1001639-37-7P   1001639-38-8P   1001639-39-9P
     1001639-41-3P   1001639-43-5P   1001639-46-8P   1001639-47-9P
     1001639-50-4P   1001639-52-6P   1001639-55-9P   1001639-58-2P
     1001639-59-3P   1001639-61-7P   1001639-63-9P   1001639-64-0P
     1001639-66-2P   1001639-68-4P   1001639-71-9P   1001639-80-0P
     1001639-89-9P   1001639-93-5P   1001639-95-7P   1001640-05-6P
     1001640-06-7P 1001640-10-3P   1001640-24-9P
     1001898-97-0P 1001898-98-1P 1001899-01-9P
     1001899-70-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of pyridazine and phthalazine derivs. of iptycenes,
        11[1',2']benzenonaphtho[2,3-d]pyridazine,
        6,11[1',2']benzenonaphtho[2,3-g]phthalazine derivs.)
IT   1001639-89-9P 1001640-06-7P 1001640-10-3P
     1001898-98-1P 1001899-01-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of pyridazine and phthalazine derivs. of iptycenes,
        11[1',2']benzenonaphtho[2,3-d]pyridazine,
        6,11[1',2']benzenonaphtho[2,3-g]phthalazine derivs.)
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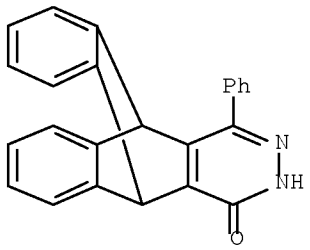
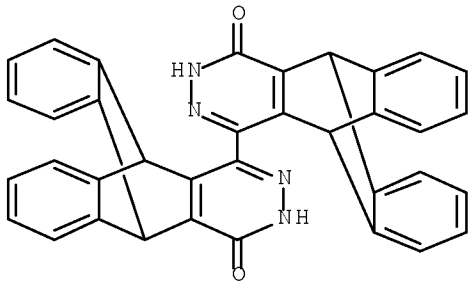
RN 1001639-89-9 HCAPLUS
CN 5,10[1',2']-Benzenobenzo[g]phthalazin-1(2H)-one, 5,10-dihydro-4-phenyl- (CA INDEX NAME)

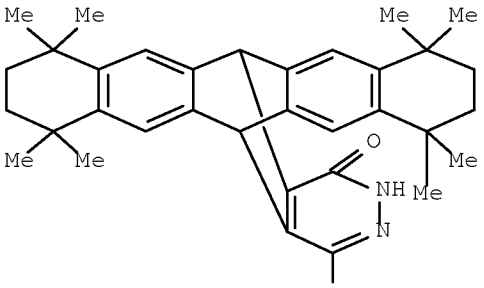


RN 1001640-06-7 HCAPLUS
CN [1,1'-Bi-5,10[1',2']-benzenobenzo[g]phthalazine]-4,4'(3H,3'H)-dione, 5,5',10,10'-tetrahydro- (CA INDEX NAME)

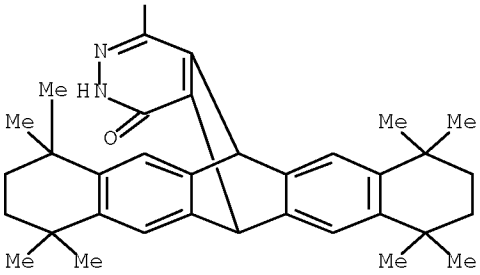


RN 1001640-10-3 HCAPLUS
CN [1,1'-Bi-5,12[2',3']-naphthalenonaphtho[2,3-g]phthalazine]-4,4'(3H,3'H)-dione, 5,7,8,9,10,12,16,17,18,19-decahydro-7,7,10,10,16,16,19,19-octamethyl- (CA INDEX NAME)

PAGE 1-A

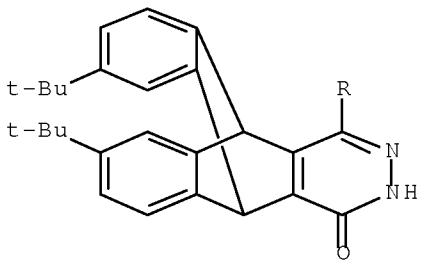


PAGE 2-A

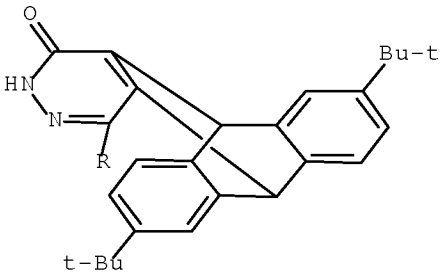


RN 1001898-98-1 HCAPLUS
CN [1,1'-Bi-5,10[1',2']-benzenobenzo[g]phthalazine]-4,4'(3H,3'H)-dione, 7,7',15,15'-tetrakis(1,1-dimethylethyl)-5,5',10,10'-tetrahydro-, stereoisomer (CA INDEX NAME)

PAGE 1-A

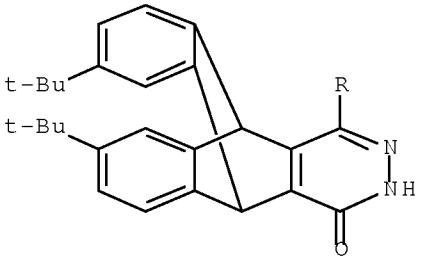


PAGE 2-A

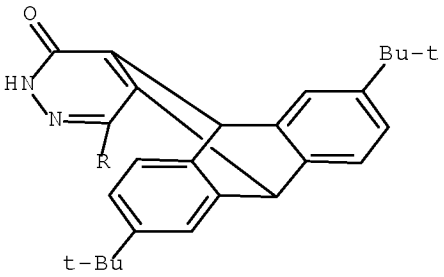


RN 1001899-01-9 HCAPLUS
CN [1,1'-Bi-5,10[1',2']-benzenobenzo[g]phthalazine]-4,4'(3H,3'H)-dione, 7,7',15,15'-tetrakis(1,1-dimethylethyl)-5,5',10,10'-tetrahydro-, stereoisomer (CA INDEX NAME)

PAGE 1-A

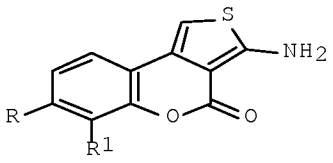


PAGE 2-A



REFERENCE COUNT: 113 THERE ARE 113 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 2 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2005:342380 HCAPLUS Full-text
DOCUMENT NUMBER: 144:88229
TITLE: Studies with condensed thiophenes: Reactivity of condensed aminothiophenes toward carbon and nitrogen electrophiles
AUTHOR(S): Al-Saleh, Balkis; Abdelkhalik, Mervat M.; El-Apasery, Morsy A.; Elnagdi, Mohamed H.
CORPORATE SOURCE: Department of Chemistry, Faculty of Science, University of Kuwait, Safat, 13060, Kuwait
SOURCE: Journal of Chemical Research (2005), (1), 23-26
CODEN: JCROA4
PUBLISHER: Science Reviews
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:88229
ED Entered STN: 21 Apr 2005
GI



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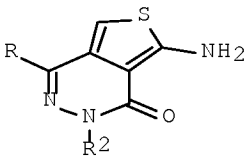


II

AB The condensed aminothiophenes I (R, R1 = H; RR1 = C4H4) and II (R = CO2Et, R2 = Ph; R = benzotriazol-1-yl, R2 = 4-MeC6H4) react with 1,4-naphthoquinone in refluxing ethanol to yield products of addition followed by hydrogen sulfide elimination in a Diels-Alder-type reaction. When the reaction is carried out under microwave irradiation a dipolar addition occurred affording products of substitution at C(1). Compds. I and II coupled with aromatic diazonium salts to yield arylazo derivs. where coupling occurred at C(1). Reaction of I and II with DMF dimethylacetal yielded amidines.

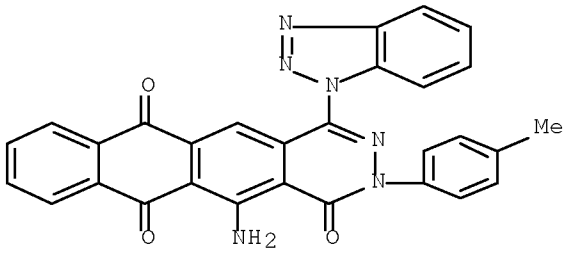
CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 872425-23-5P 872425-24-6P 872425-25-7P 872425-26-8P
872425-27-9P 872425-28-0P 872425-29-1P 872425-30-4P 872425-31-5P
872425-32-6P 872425-33-7P 872425-34-8P 872425-35-9P 872425-36-0P
872425-39-3P 872425-40-6P 872425-41-7P 872425-42-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(reactions of condensed aminothiophenes with carbon and nitrogen electrophiles)

IT 872425-25-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(reactions of condensed aminothiophenes with carbon and nitrogen electrophiles)

RN 872425-25-7 HCAPLUS

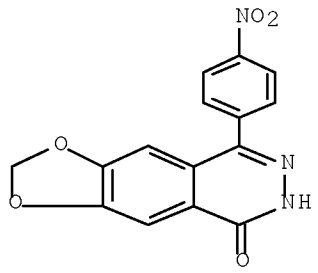
CN Naphtho[2,3-g]phthalazine-1,6,11(2H)-trione, 12-amino-4-(1H-benzotriazol-1-yl)-2-(4-methylphenyl)- (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

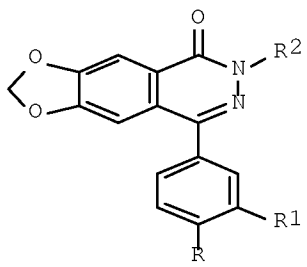
L55 ANSWER 3 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2002:224723 HCAPLUS Full-text
DOCUMENT NUMBER: 137:194982
TITLE: Triazolo- and imidazophthalazines, are they non-competitive AMPA antagonists?
AUTHOR(S): Solyom, Sandor; Hamori, Tamas; Borosy, Andras P.; Tarnawa, Istvan; Berzsenyi, Pal; Pallagi, Istvan
CORPORATE SOURCE: IVAX Drug Research Institute, Ltd, Budapest, H-1045, Hung.
SOURCE: Medicinal Chemistry Research (2002), 11(1), 39-49
CODEN: MCREEB; ISSN: 1054-2523
PUBLISHER: Birkhaeuser Boston
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:194982
ED Entered STN: 25 Mar 2002
AB Earlier structure-activity relationship studies within the 2,3-benzodiazepine family had revealed that the 3-acyl-4-Me part of 2, an active non-competitive AMPA antagonist, can be substituted by condensed azolenings at the same position preserving or improving biol. activity. This suggests that the same structural features can be applied to some phthalazine derivs. that have been shown to possess non-competitive AMPA antagonist activity. Therefore new [1,2,4]triazolo[3,4-a]- and imidazo[2,1-a]phthalazines of type 21 were synthesized applying known and new methods in multistep routes. The resulted compds. had no pharmacol. activity either in vitro (up to 20 μM) or in vivo (up to 100 mg/kg i.p., or 200 mg/kg orally). To find a possible explanation for the lack of AMPA antagonistic potencies a computer aided mol. modeling study was performed.
CC 1-3 (Pharmacology)
Section cross-reference(s): 27
IT 295793-38-3P 452973-84-1P 452973-85-2P 452973-86-3P
452973-87-4P 452973-88-5P 452973-89-6P 452973-90-9P 452973-91-0P
452973-92-1P 452973-93-2P 452973-94-3P 452973-95-4P 452973-96-5P
452973-97-6P 452973-98-7P 452973-99-8P 452974-00-4P 452974-01-5P
452974-02-6P 452974-03-7P 452974-04-8P 452974-05-9P 452974-06-0P
452974-07-1P 452974-08-2P 452974-09-3P 452974-10-6P 452974-11-7P
452974-12-8P 452974-13-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(triazolo- and imidazophthalazines, are they non-competitive AMPA antagonists)
IT 295793-38-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(triazolo- and imidazophthalazines, are they non-competitive AMPA antagonists)
RN 295793-38-3 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-nitrophenyl)- (CA INDEX NAME)



REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 4 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 2000:457925 HCAPLUS Full-text
DOCUMENT NUMBER: 133:246792
TITLE: Synthesis and anticonvulsant activity of novel and potent 6,7-methylenedioxyphthalazin-1(2H)-ones
AUTHOR(S): Grasso, Silvana; De rro, Giovambattista; De Sarro, Angela; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; De icheli, Carlo
CORPORATE SOURCE: Dipartimento Farmaco-Chimico and Istituto di Farmacologia, Universita di Messina, Messina, Italy
SOURCE: Journal of Medicinal Chemistry (2000), 43(15), 2851-2859
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:246792
ED Entered STN: 09 Jul 2000
GI



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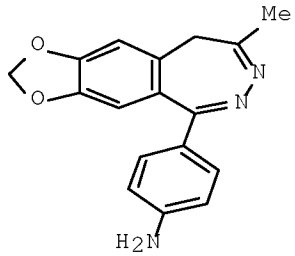


II

AB In this paper, the authors describe the synthesis of a series of novel substituted 4-aryl-6,7-methylenedioxyphthalazin-1(2H)-ones I (R = H, O2N, H2N; R1 = H, O2N, H2N; R2 = H, R3NHCO; R3 = Me, Et, EtCH2, Bu, BuCH2, cyclohexyl). The anticonvulsant activity of these compds. against audiogenic seizures was evaluated in DBA/2 mice after i.p. (i.p.) injection. Most of these derivs. are more active than 1-(4-aminophenyl)-4-methyl-7,8-methylenedioxy-5H-2,3-benzodiazepine II (GYKI 52466), a well-known noncompetitive AMPA receptor antagonist. As deduced by the rotarod test, all the compds. exhibit a toxicity lower than that of II. Within the series of derivs. submitted to investigation, 4-(4-aminophenyl)-2-butylcarbamoyl-6,7-methylenedioxyphthalazin-1(2H)-one I (R = H2N; R1 = H; R2 = BuNHCO) proved to be the most active compound and is 11-fold more potent than II [i.e., ED50 3.25 μmol/kg for I (R = H2N; R1 = H; R2 = BuNHCO) vs. ED50 35.8 μmol/kg for II]. When compared to II, compound I (R = H2N; R1 = H; R2 = BuNHCO) as well as its analog 4-(4-aminophenyl)-6,7-methylenedioxyphthalazin-1(2H)-one I (R = H2N; R1 = R2 = H) show a longer lasting anticonvulsant activity. Compound I (R = H2N; R1 = H; R2 = BuNHCO) also effectively suppresses seizures induced in Swiss mice by maximal electroshock (MES) and pentylenetetrazole (PTZ). Furthermore, it antagonizes in vivo seizures induced by 2-amino-3-(3-hydroxy-5-methylisoxazol-4-yl)propionic acid (AMPA), 2-amino-3-(3-hydroxy-5-tert-butylisoxazol-4-yl)propionic acid (ATPA), and kainate (KA), and its anticonvulsant activity is reversed by pretreatment with aniracetam. Using the patch-clamp technique, the capability of derivs. III and IV to antagonize KA-evoked currents in primary cultures of granule neurons was tested. They behaved as antagonists, but they proved to be less effective than II and 1-(4-aminophenyl)-3,4-dihydro-4-methyl-3- N-methylcarbamoyl-7,8-methylene dioxy-5H-2,3-benzodiazepine (GYKI 53655) to reduce the KA-evoked currents.

CC 1-3 (Pharmacology)
Section cross-reference(s): 28

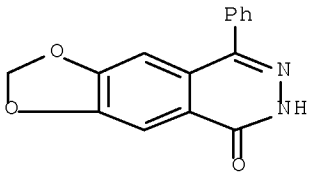
IT 295793-36-1P 295793-37-2P 295793-38-3P
295793-40-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation and anticonvulsant activity of (methylenedioxy)phthalazinones)

IT 295793-39-4P 295793-41-8P 295793-42-9P
295793-43-0P 295793-44-1P 295793-45-2P
295793-46-3P 295793-47-4P 295793-48-5P
295793-49-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and anticonvulsant activity of (methylenedioxy)phthalazinones)

IT 295793-36-1P 295793-37-2P 295793-38-3P
295793-40-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation and anticonvulsant activity of (methylenedioxy)phthalazinones)

RN 295793-36-1 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-phenyl- (CA INDEX NAME)



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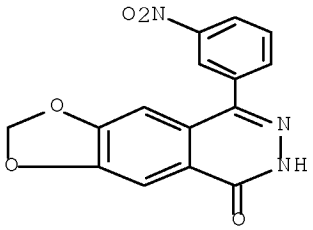
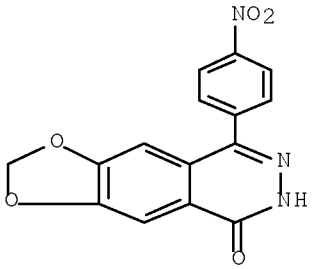


RN 295793-38-3 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-nitrophenyl)- (CA INDEX NAME)



RN 295793-40-7 HCAPLUS
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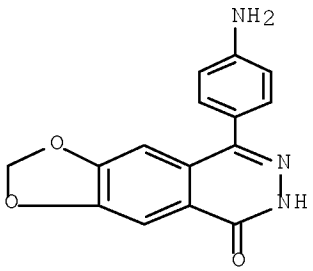
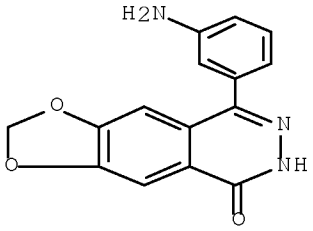
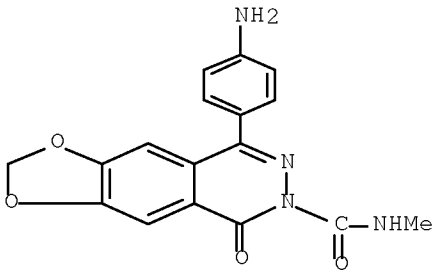


IT 295793-39-4P 295793-41-8P 295793-42-9P
295793-43-0P 295793-44-1P 295793-45-2P
295793-46-3P 295793-47-4P 295793-48-5P
295793-49-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and anticonvulsant activity of (methylenedioxy)phthalazinones)
RN 295793-39-4 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(3-aminophenyl)- (CA INDEX NAME)

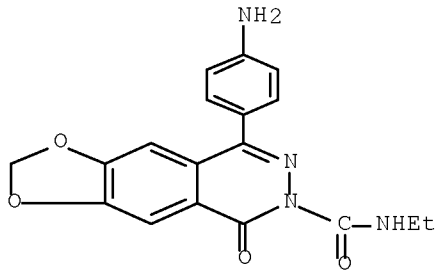


RN 295793-41-8 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide, 8-(4-aminophenyl)-N-methyl-5-oxo- (CA INDEX NAME)

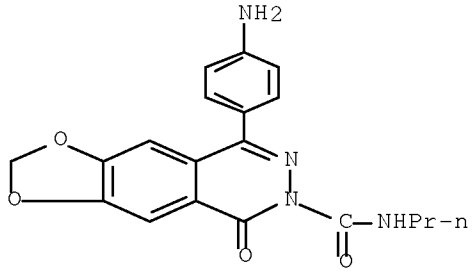


RN 295793-42-9 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide,

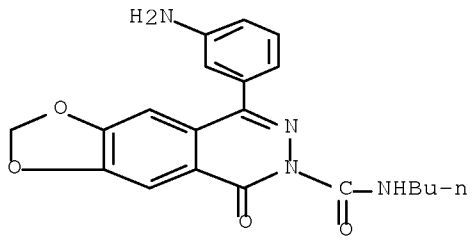
8-(4-aminophenyl)-N-ethyl-5-oxo- (CA INDEX NAME)



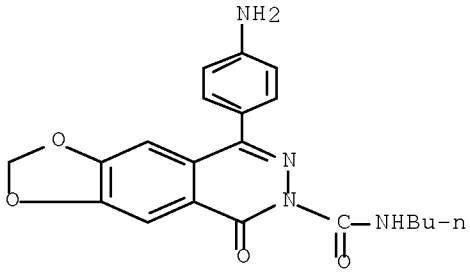
RN 295793-43-0 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide,
8-(4-aminophenyl)-5-oxo-N-propyl- (CA INDEX NAME)



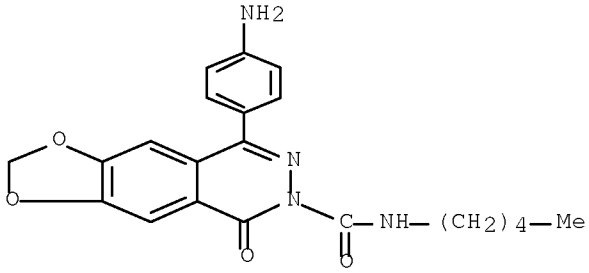
RN 295793-44-1 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide,
8-(3-aminophenyl)-N-butyl-5-oxo- (CA INDEX NAME)



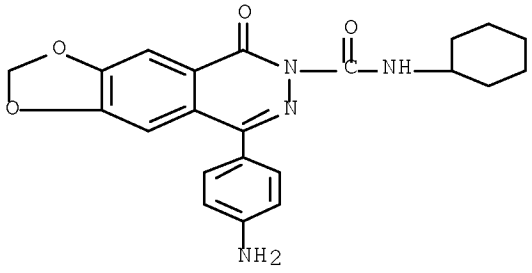
RN 295793-45-2 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide,
8-(4-aminophenyl)-N-butyl-5-oxo- (CA INDEX NAME)



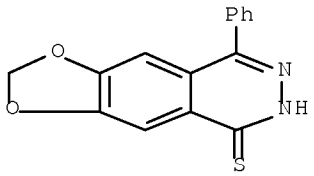
RN 295793-46-3 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide,
8-(4-aminophenyl)-5-oxo-N-pentyl- (CA INDEX NAME)



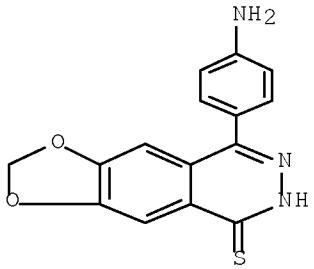
RN 295793-47-4 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide,
8-(4-aminophenyl)-N-cyclohexyl-5-oxo- (CA INDEX NAME)



RN 295793-48-5 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazine-5(6H)-thione, 8-phenyl- (CA INDEX NAME)

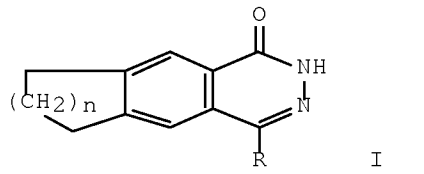


RN 295793-49-6 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazine-5(6H)-thione, 8-(4-aminophenyl)- (CA INDEX NAME)



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 5 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 1995:956557 HCAPLUS Full-text
DOCUMENT NUMBER: 124:146037
ORIGINAL REFERENCE NO.: 124:27161a,27164a
TITLE: Inverse-electron-demand Diels-Alder reactions of condensed pyridazines. 8. Convenient synthesis of cycloalkene-fused phthalazinones
AUTHOR(S): Haider, Norbert
CORPORATE SOURCE: Inst. Pharmaceutical Chem., Univ. Vienna, Vienna, A-1090, Austria
SOURCE: Heterocycles (1995), 41(11), 2519-25
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:146037
ED Entered STN: 01 Dec 1995
GI



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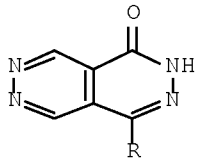
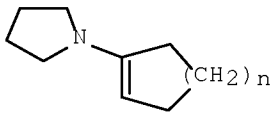


II



III

AB A series of cycloalkene-annulated phthalazin-1(2H)-ones I (R = Et, Ph, n = 1-4) was prepared in high yields by a one-pot procedure, employing pyridazino[4,5-d]pyridazin-1(2H)-ones II as azadienes and cyclic enamines III as dienophiles in an inverse-electron-demand Diels-Alder reaction, followed by acid-catalyzed aromatization.

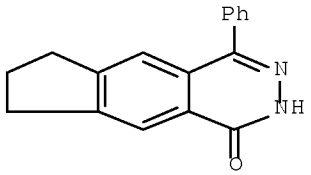
CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 173463-56-4P 173463-57-5P 173463-58-6P 173463-59-7P
173463-60-0P 173463-61-1P 173463-62-2P 173463-63-3P 173463-64-4P
173463-65-5P 173463-66-6P 173463-67-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of cycloalkene-fused phthalazinones by Diels-Alder of condensed
pyridazines with cyclic enamines)

IT 173463-57-5P 173463-59-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of cycloalkene-fused phthalazinones by Diels-Alder of condensed
pyridazines with cyclic enamines)

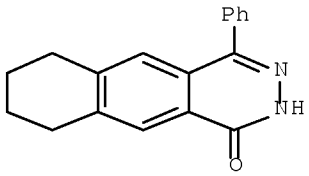
RN 173463-57-5 HCAPLUS

CN 1H-Cyclopenta[g]phthalazin-1-one, 2,6,7,8-tetrahydro-4-phenyl- (CA INDEX NAME)



RN 173463-59-7 HCAPLUS

CN Benzo[g]phthalazin-1(2H)-one, 6,7,8,9-tetrahydro-4-phenyl- (CA INDEX NAME)



L55 ANSWER 6 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 6
ACCESSION NUMBER: 1958:87985 HCAPLUS Full-text
DOCUMENT NUMBER: 52:87985
ORIGINAL REFERENCE NO.: 52:15485g-i,15486a-i
TITLE: Selective reduction by calcium hexammine. I. Aromatic hydrocarbons
AUTHOR(S): Boer, H.; Duinker, P. M.
CORPORATE SOURCE: Roy. Shell Lab., Amsterdam
SOURCE: Recueil des Travaux Chimiques des Pays-Bas et de la Belgique (1958), 77, 346-59
CODEN: RTCPB4; ISSN: 0370-7539
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 52:87985
ED Entered STN: 22 Apr 2001
AB Under carefully adjusted reaction conditions polynuclear aromatic hydrocarbons were selectively reduced by Ca(NH3)6 (I) to compds. containing only one isolated benzene ring. The hydrocarbons used were purified com. or synthetic samples and the details of synthesis and phys. properties are tabulated. Carefully dried liquid NH3 and a known weight of Ca chips siphoned under N into an Et2O solution of hydrocarbon (30 millimoles/100 ml. Et2O), the mixture stirred vigorously with evaporation of the NH3, kept 23 hrs., filtered (N atm) without suction, and the filtrate evaporated gave a clear residue of product. Ca powder in Et2O at 0° saturated with a slight excess of NH3, the hydrocarbon added carefully (4 moles NH3 liberated by 1 mole reactive I), and the mixture worked up as above gave the reduced product. Ca was calculated on the basis of conversion of polyaromatics to monoaromatics with 50% excess and recoveries were generally better than 95%. Details of general methods for determining the reaction products by catalytic hydrogenation, percolation, ultraviolet spectroscopy, gas-liquid chromatography, ozonometry, and refractive index detns. are given. Comparison of the ultraviolet spectra before and after catalytic hydrogenation showed conjugated cyclohexadienes to be absent in the reaction products of alkylbenzenes on reduction by the "liquid ammonia" method. In a few expts. the product was percolated over silica and the absence of alkylcyelohexanes demonstrated. From the total unsatn., determined ozonometrically, and the amount of unreacted aromatics, as found by ultraviolet spectral analysis after hydrogenation, the contents of alkylcyclohexene and alkylcyclohexadiene were calculated and the data obtained confirmed by refractive index analyses. Results of the "liquid ammonia" reduction of alkylbenzenes are tabulated (hydrocarbon, weight-% unreacted, weight-% cyclohexadienes, and weight-% cyclohexenes given): C6H6, -, -, 100; PhMe, 10, 32, 58; PhEt, 19, 21, 60; o-xylene, 68, 17, 15; m-xylene, 30, 35, 35; p-xylene, 42, 40, 18. Reduction of 1,2,4- and 1,3,5-C6H3Me3, 1,2,4,5-C6H2Me4, and C6Me6 gave 86, 72, 94, and 100% unreacted material and 14, 28, 6, and 0% unidentified mixts. of cyclohexadienes and cyclohexenes. A number of compds. containing more than one aromatic ring were treated with I by the same procedure (polynuclear aromatic, weight-% monoaromatics, and weight-% nonaromatic cycloalkenes given): Ph2, 55, 45; Ph2CH2, 56, 44; C10H8, 40, 60;

anthracene, -, 100; phenanthrene, 42, 58; 1-methyl-7-isopropylphenanthrene, 85, 15; triphenylene, 63, 37. Thus, the polynuclear aromatics are quantitatively reduced to benzene derivs. which may undergo partial reduction to cycloalkenes. In a series of reductions of 1,2,3,4-tetrahydronaphthalene by the "gaseous ammonia" method it was shown that the C6H6 nucleus was but very little attacked at 0° in 1 hr. The results of reduction of various polynuclear aromatics under these conditions are summarized [aromatic, weight-% unreacted, weight-% benzene derivs. (composition of monoaromatic fraction) and weight-% nonaromatic cycloalkenes given]: Ph2, 0.4, 99 (21% phenylcyclohexene and 79% phenylcyclohexane), -; Ph2CH2, 84, 16 (phenylcyclohexenylmethane and phenylcyclohexadienylmethane), -; (PhCH2)2, 95, 5 (PhCH2CH2C6H9), -; C10H8, -, 94 (1,2,3,4-tetrahydronaphthalene), 6 (mainly C10H16); acenaphthene, trace, 100 (tetrahydroacenaphthene), -; 2,3,6-Me3C10H5, 1, 99 (8% trimethyltetrahydronaphthalene, 92% 1,4-dihydrotrimethylnaphthalene), -; anthracene, 0.17, - (9,10-dihydro- and hexahydroanthracene), -; phenanthrene, trace, 100 (7% hexahydrophenanthracene), -; phenanthrene, trace, 100 (7% hexa- and 93% octahydrophenanthrene), -. To demonstrate that alkenylbenzenes with a side-chain containing a double bond in conjunction with the aromatic nucleus are readily reduced with I, comparative reductions with Tetralin were made (compound, weight-% unreacted, weight-% indan, weight-% PhEt, and weight-% nonaromatic cycloalkenes given): indene, 30, 54, -, 15.5; styrene, -, -, 94, 2; indan, 90, 90, -, 8; Tetralin, 95, -, -, 5. It would appear that the reduction of indene to a nonaromatic cycloalkene takes place via an intermediate other than indan. The selectivity of I reduction made possible the preparation of compds. previously difficult to synthesize. Ground Ca (80 g.) in 1 l. dry Et2O at 0° saturated with a stream of dry NH3 (60 l./hr.) and diluted with 156 g. dry C6H6, the cooling bath removed, the NH3 evaporated 1.5 hrs., the residue acidified at -20°, and the washed and dried Et2O layer evaporated gave 142 g. product, n25D 1.4721 (containing 0.945 alkene-type double bond/mol.), converted to the tetrabromide and washed with hot MeOH; the mixture of 2 stereoisomeric tetrabromides, m. 176-81°, decomposed according to Huckel and Worffel (C.A. 50, 7093e) yielded 30% pure 1,4-cyclohexadiene, b774 88.7-9.1°, n20D 1.4722. Dry NH3 gas (30 l./hr.) passed 4 hrs. into 1 l. dry ether stirred with 60 g. powdered Ca and 60 g. phenanthrene, the mixture suction-filtered, the filter cake added portionwise to H2O, and the acidified solution extracted with Et2O gave 185 g. (3 consecutive prepns.) containing 9% alkene compds. The material hydrogenated at 100°/200 atmospheric with Cu chromite catalyst, and the product percolated over silica and Al2O3 gave 176 g. octahydrophenanthrenes, n25D 1.5575, distilled over a 20-theoretical plate Vigreux column to show the presence of 45% sym. and 55% unsym. isomers, n25D 1.5461 and 1.5513, resp. Mixts. of alkyl-substituted Tetralins (II) were obtained from the alkylnaphthalenes by the "gaseous ammonia" technique and worked up as above; α- and β-methylnaphthalenes gave only II whereas the reaction product of 2,3-C10H6Me2 contained 14% aliphatic double bonds. Some remarks are made on the mechanism of the reaction.

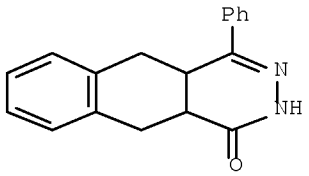
CC 10 (Organic Chemistry)

IT 12133-31-2 29811-05-0 76044-99-0 101723-54-0 101789-59-7 109892-05-9 114722-26-8
(Derived from data in the 6th Collective Formula Index (1957-1961))

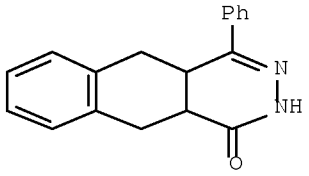
IT 109892-05-9
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 109892-05-9 HCAPLUS

CN Benzo[g]phthalazin-1(2H)-one, 4a,5,10,10a-tetrahydro-4-phenyl- (CA INDEX NAME)

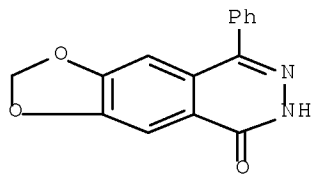


L55 ANSWER 7 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 7
ACCESSION NUMBER: 1958:87986 HCAPLUS Full-text
DOCUMENT NUMBER: 52:87986
ORIGINAL REFERENCE NO.: 52:15486i,15487a
TITLE: Unsaturated hydrocarbons. III. New method of synthesis of aromatic hydrocarbons with a desired structure
AUTHOR(S): Kotlyarevskii, I. L.; Zanina, A. S.; Lipovich, V. G.
SOURCE: Zhurnal Prikladnoi Khimii (Sankt-Peterburg, Russian Federation) (1957), 30, 335-7
CODEN: ZPKHAB; ISSN: 0044-4618
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 22 Apr 2001
AB See C.A. 51, 13790i.
CC 10 (Organic Chemistry)
IT 1559-81-5 1680-51-9 2809-64-5 3877-19-8 29811-05-0 76044-99-0 101723-54-0 101789-59-7 109892-05-9 114722-26-8
(Derived from data in the 6th Collective Formula Index (1957-1961))
IT 109892-05-9
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 109892-05-9 HCAPLUS
CN Benzo[g]phthalazin-1(2H)-one, 4a,5,10,10a-tetrahydro-4-phenyl- (CA INDEX NAME)

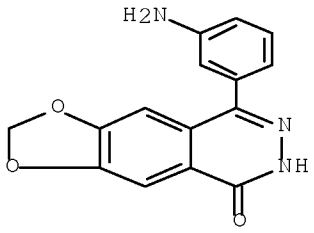


L55 ANSWER 8 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:430641 HCAPLUS Full-text
DOCUMENT NUMBER: 143:165974
TITLE: QSAR study of 2,3-benzodiazepin-4(thi)one- and 1,2-phthalazine-related negative allosteric modulators of the AMPA receptor: A structural descriptors-based reassessment
AUTHOR(S): Buchwald, Peter; Einstein, Brandon; Bodor, Nicholas
CORPORATE SOURCE: IVAX Research, Inc., Miami, FL, USA
SOURCE: QSAR & Combinatorial Science (2005), 24(3), 325-331
CODEN: QCSSAU; ISSN: 1611-020X
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

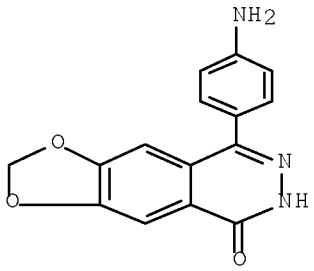
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 20 May 2005
AB In an attempt to establish statistically more rigorous and chemical more meaningful quant. structure-activity relationship (QSAR) equations, a reassessment of a recent study of in vivo anticonvulsant activity for a set of 2,3-benzodiazepin-4(thi)one- and 1,2-phthalazine-related allosteric AMPA antagonists (n=61) is presented. Contrary to the original, relatively nonspecific descriptor set, which included, for example, a number of topol. descriptors, specific structural descriptors that are much easier to interpret from a medicinal chemical point of view are used in this multiple linear regression-based approach. Only statistically significant descriptors have been retained in the final equation, and whereas they give about the same correlation as those of the original paper on the training set (r2 of 0.79 vs. 0.76, n=49), they perform much better on the test set (predictive r2pr of 0.73 vs. 0.05; r2 of 0.78 vs. 0.08, n=12). Descriptors found to be relevant are clearly related to substitutions at known pharmacophore positions, such as those corresponding to the 2,3-, 7,8- and 4'-positions of the benzodiazepine skeleton. Therefore, by a more careful selection of the descriptor set, both an improved prediction and a more intuitive quant. interpretation could be achieved for this set of allosteric AMPA antagonists.
CC 1-3 (Pharmacology)
IT 35011-63-3 41148-41-8 41148-42-9 47281-61-8 55507-15-8
96315-84-3 96315-85-4 102693-05-0 102693-13-0 102693-14-1
102693-24-3 173284-36-1 178616-26-7 187940-09-6 187940-20-1
187940-28-9 187940-29-0 187940-30-3 187940-31-4 187940-33-6
197368-44-8 197368-47-1 197368-49-3 197368-51-7 197368-92-6
197369-07-6 213385-71-8 213385-72-9 213385-73-0 213385-74-1
213385-76-3 213385-77-4 213385-78-5 213385-79-6 213385-80-9
213385-81-0 231623-78-2 236109-55-0 236109-57-2 236109-58-3
250699-34-4 250699-41-3 292858-36-7 292858-38-9 292858-39-0
292858-40-3 292858-42-5 292858-46-9 295793-36-1
295793-39-4 295793-40-7 295793-41-8
295793-43-0 320349-99-3 320350-01-4 320350-02-5
320350-03-6 320350-04-7 320350-05-8 320350-06-9 681457-29-4
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(OSAR study of 2,3-benzodiazepin-4(thi)one- and 1,2-phthalazine-related neg. allosteric modulators of AMPA receptor and a structural descriptors-based reassessment)
IT 295793-36-1 295793-39-4 295793-40-7
295793-41-8 295793-43-0
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(OSAR study of 2,3-benzodiazepin-4(thi)one- and 1,2-phthalazine-related neg. allosteric modulators of AMPA receptor and a structural descriptors-based reassessment)
RN 295793-36-1 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-phenyl- (CA INDEX NAME)



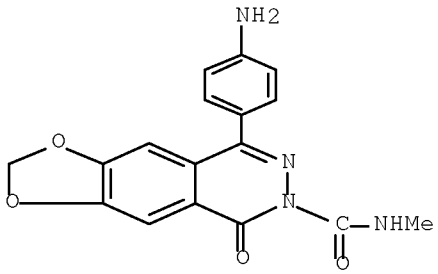
RN 295793-39-4 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(3-aminophenyl)- (CA INDEX NAME)



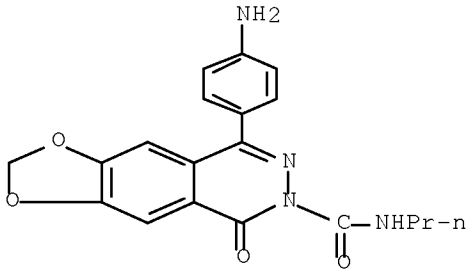
RN 295793-40-7 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-aminophenyl)- (CA INDEX NAME)



RN 295793-41-8 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide, 8-(4-aminophenyl)-N-methyl-5-oxo- (CA INDEX NAME)



RN 295793-43-0 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide, 8-(4-aminophenyl)-5-oxo-N-propyl- (CA INDEX NAME)

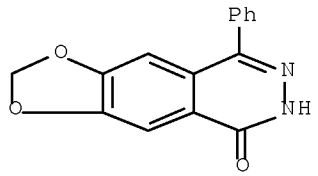


REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

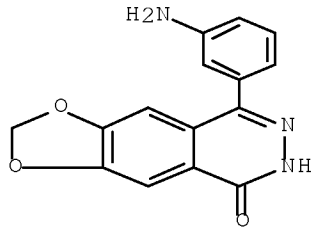
L55 ANSWER 9 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:168622 HCAPLUS Full-text
DOCUMENT NUMBER: 140:350044
TITLE: QSAR Study of Anticonvulsant Negative Allosteric Modulators of the AMPA Receptor
AUTHOR(S): Macchiarulo, Antonio; De Luca, Laura; Costantino, Gabriele; Barreca, Maria Letizia; Gitto, Rosaria; Pellicciari, Roberto; Chimirri, Alba
CORPORATE SOURCE: Dipartimento di Chimica e Tecnologia del Farmaco, Universita di Perugia, Perugia, 06123, Italy
SOURCE: Journal of Medicinal Chemistry (2004), 47(7), 1860-1863
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 02 Mar 2004
AB A quant. structure-activity relation (QSAR) study was performed on a set of 49 neg. allosteric modulators of AMPA receptor, acting as anticonvulsant agents, using multiple linear regression. The predictive ability of the resulting model was evaluated against a set of 12 compds.; the results showed good statistics in regression and revealed high correlation between anticonvulsant activity and some electrotopol. descriptors.
CC 1-3 (Pharmacology)
IT 41148-41-8 41148-42-9 47281-61-8 55507-15-8 96315-84-3
96315-85-4 102693-05-0 102693-13-0 102693-14-1 102693-24-3
102771-26-6 173284-36-1 178616-26-7 187940-09-6 187940-20-1
187940-28-9 187940-29-0 187940-30-3 187940-31-4 187940-33-6
197368-44-8 197368-47-1 197368-49-3 197368-51-7 197368-92-6
197369-07-6 213385-71-8 213385-72-9 213385-73-0 213385-74-1
213385-76-3 213385-77-4 213385-78-5 213385-79-6 213385-80-9
213385-81-0 231623-78-2 236109-55-0 236109-57-2 236109-58-3
250699-34-4 250699-41-3 292858-36-7 292858-38-9 292858-39-0
292858-40-3 292858-42-5 292858-46-9 295793-36-1
295793-39-4 295793-40-7 295793-41-8
295793-43-0 320349-99-3 320350-01-4 320350-02-5
320350-03-6 320350-04-7 320350-05-8 320350-06-9 681457-29-4
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR of anticonvulsant neg. allosteric modulators of AMPA receptor)
IT 295793-36-1 295793-39-4 295793-40-7

295793-41-8 295793-43-0
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR of anticonvulsant neg. allosteric modulators of AMPA receptor)

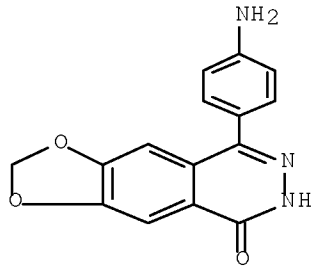
RN 295793-36-1 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-phenyl- (CA INDEX NAME)



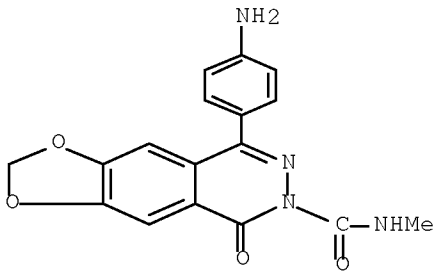
RN 295793-39-4 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(3-aminophenyl)- (CA INDEX NAME)



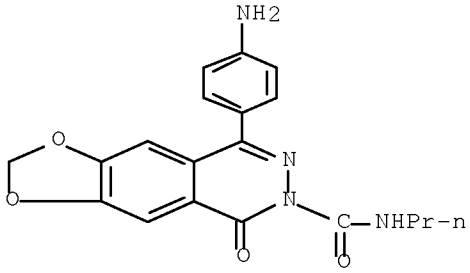
RN 295793-40-7 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-aminophenyl)- (CA INDEX NAME)



RN 295793-41-8 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide, 8-(4-aminophenyl)-N-methyl-5-oxo- (CA INDEX NAME)



RN 295793-43-0 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide, 8-(4-aminophenyl)-5-oxo-N-propyl- (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 10 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:205961 HCAPLUS Full-text
DOCUMENT NUMBER: 142:197900
TITLE: Product class 10: phthalazines
AUTHOR(S): Haider, N.; Holzer, W.
CORPORATE SOURCE: Germany
SOURCE: Science of Synthesis (2004), 16, 315-372
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
ED Entered STN: 15 Mar 2004
AB A review. Preparation is given for phthalazines via ring closure or transformation reactions, aromatization or substituent modification.
CC 28-0 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 66645-92-9 66859-13-0 67081-02-1 70097-45-9 70801-31-9
70801-33-1 73661-77-5 73661-78-6 73661-79-7 75998-18-4
76240-43-2 76972-35-5 79690-84-9 84641-77-0 86355-12-6
87255-76-3 89516-24-5 90719-21-4 90915-39-2 91054-33-0
91566-88-0 92722-88-8 95884-14-3 97694-85-4 99161-49-6
100448-45-1 100448-46-2 100537-30-2 101440-97-5 101889-52-5
105850-89-3 112633-87-1 112633-89-3 114202-92-5 119838-09-4
121561-18-0 122665-83-2 124433-93-8 129221-76-7 132960-21-5
137207-61-5 137207-65-9 137382-32-2 137382-37-7 143915-58-6
153078-00-3 153078-01-4 155937-09-0 155937-30-7 161851-52-1

170373-53-2 178309-37-0 183968-10-7 189213-58-9 210166-63-5
210166-73-7 219966-12-8 219966-14-0 226995-83-1 295793-36-1
297132-06-0 297132-07-1 297132-08-2 311339-02-3 350690-07-2
412339-50-5 479058-74-7 537033-42-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phthalazines)

IT 119-39-1P, 1(2H)-Phthalazinone 253-52-1P, Phthalazine 484-23-1P
1445-69-8P 2257-69-4P 4673-39-6P 4752-10-7P 5004-45-5P
5004-46-6P 5004-48-8P 5784-45-2P 7624-86-4P 10001-35-1P
10132-01-1P 13925-27-4P 14503-64-1P 15994-75-9P 16015-46-6P,
1(2H)-Phthalazinethione 17341-79-6P 17987-70-1P,
1,4-Phthalazinediamine 19064-69-8P, 1-Phthalazinamine 21131-44-2P
21452-56-2P 21948-74-3P 25947-13-1P 35392-60-0P 38710-51-9P
39794-30-4P 40125-48-2P 40848-53-1P 51793-94-3P 54145-23-2P
57835-96-8P 63536-21-0P 68775-89-3P 75884-68-3P 75884-74-1P
77533-21-2P 81731-69-3P 89891-73-6P 89898-86-2P 90754-78-2P
91587-99-4P 94309-83-8P 100881-26-3P 101094-85-3P 103286-03-9P
103286-04-0P 105936-84-3P 107558-48-5P 107559-06-8P 128066-18-2P
154822-28-3P 154822-30-7P 154822-32-9P 154822-34-1P 155937-32-9P
167705-73-9P 173463-59-7P 203929-42-4P 203929-43-5P
203929-44-6P 203929-45-7P 203929-47-9P 203929-49-1P 203929-51-5P
203929-53-7P 203929-55-9P 203929-56-0P 203929-58-2P 203929-61-7P
203929-63-9P 203929-65-1P 203929-66-2P 203929-68-4P 203929-70-8P
221632-73-1P 221632-74-2P 221632-75-3P 221632-77-5P 228869-44-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of phthalazines)

IT 86-54-4P 269-50-1P, 1,3-Dioxolo[4,5-g]phthalazine 1133-73-9P
2258-88-0P 3306-76-1P 3682-15-3P 4776-85-6P 4870-16-0P
5439-98-5P 5441-28-1P 6091-81-2P 6266-49-5P 6941-96-4P
7188-22-9P 10089-99-3P 10132-02-2P 10132-05-5P 13580-85-3P
13580-86-4P 13580-88-6P 13705-95-8P 14062-52-3P 14161-35-4P
16676-79-2P 17045-94-2P 17045-95-3P 18393-54-9P 18496-20-3P
18584-50-4P 18584-52-6P 18584-53-7P 18584-54-8P 18636-89-0P
18640-46-5P 18697-31-9P 21948-84-5P 23100-01-8P 24129-03-1P
24129-10-0P 24953-61-5P 24953-63-7P 24953-64-8P 24953-65-9P
25131-53-7P 25732-39-2P 25732-41-6P 25732-42-7P 26238-15-3P
26641-43-0P 28081-56-3P 29415-71-2P 29902-28-1P 36503-83-0P
38933-79-8P 39794-28-0P 39794-29-1P 39998-72-6P 41886-43-5P
49572-99-8P 51334-85-1P 51935-42-3P 54145-30-1P 57413-62-4P
57835-94-6P 59283-65-7P 59908-32-6P 60889-20-5P 61503-69-3P
62645-07-2P 63536-23-2P 63536-29-8P 63536-30-1P 63536-31-2P
63536-36-7P 66859-14-1P 68775-90-6P 68775-92-8P 71271-35-7P
73662-08-5P 73662-09-6P 73662-10-9P 76240-45-4P 76240-46-5P
76240-47-6P 76462-35-6P 76462-36-7P 76870-65-0P 76972-37-7P
76972-84-4P 76972-85-5P 81214-62-2P 81731-72-8P 82908-72-3P
82908-80-3P 84257-71-6P 86355-25-1P 87166-52-7P 87166-60-7P
87166-61-8P 87255-77-4P 89898-93-1P 89898-94-2P 89898-95-3P
89939-65-1P 90876-71-4P 93517-74-9P 93517-75-0P 93517-76-1P
93517-77-2P 94106-83-9P 95647-35-1P 97694-84-3P 97694-87-6P
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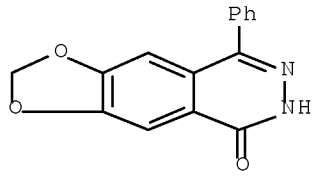
99161-51-0P 99185-48-5P 100139-18-2P 100330-23-2P 100448-25-7P
100448-26-8P 100448-27-9P 100448-47-3P 100448-48-4P 100448-50-8P
100541-08-0P 100962-00-3P 101494-94-4P 101495-53-8P 101721-36-2P
102072-84-4P, 5-Phthalazinamine 103038-14-8P 103286-05-1P
103286-06-2P 103286-07-3P 103286-08-4P 103286-11-9P 103286-12-0P
103286-26-6P 103286-28-8P 103286-29-9P 103286-30-2P 104819-04-7P
105702-06-5P 108618-32-2P 110175-26-3P 110704-04-6P 112633-90-6P
112633-91-7P 113222-30-3P 121258-89-7P 121561-21-5P 122665-86-5P
122665-88-7P 124397-50-8P 124433-94-9P 124556-68-9P 124556-78-1P

126081-03-6P 126278-18-0P 126650-65-5P 129221-92-7P 132960-22-6P
132960-23-7P 134926-55-9P 134926-67-3P 134926-68-4P 135033-30-6P
135033-31-7P 135033-32-8P 135033-33-9P 135033-34-0P 135033-35-1P
136610-31-6P 136610-32-7P 136610-33-8P 137207-76-2P 137381-09-0P
137381-69-2P 137382-01-5P 137382-07-1P 137382-08-2P 137382-09-3P
137382-45-7P 137382-60-6P 137387-90-7P 155936-76-8P 155936-78-0P
155937-28-3P 156020-35-8P 159211-19-5P 163120-65-8P 163120-66-9P
170373-52-1P 170940-78-0P, 1-Phthalazinecarboxamide 171084-38-1P
171084-39-2P 173463-56-4P 173463-57-5P 173463-58-6P
173463-60-0P 173463-61-1P 173463-62-2P 173463-63-3P 173605-15-7P
178309-35-8P 178309-36-9P 180293-88-3P 182683-72-3P 184474-93-9P
189213-64-7P 201531-14-8P 203929-72-0P 203929-74-2P 203929-76-4P
203929-77-5P 203929-78-6P 203929-79-7P 203929-80-0P 203929-81-1P
203929-82-2P 203929-83-3P 203929-84-4P 203929-85-5P 203929-86-6P
203929-87-7P 203929-88-8P 203929-89-9P 203929-90-2P 203929-91-3P
204520-35-4P 210166-64-6P 210166-74-8P 212141-54-3P 212141-72-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of phthalazines)

IT 212142-91-1P 212142-96-6P 213765-59-4P 219966-13-9P 220411-63-2P
220411-64-3P 220411-65-4P 220411-66-5P 220411-67-6P 220411-68-7P
221632-80-0P 221632-81-1P 221632-83-3P 221632-85-5P 221632-86-6P
226385-58-6P 226385-61-1P 226385-64-4P 226385-65-5P 226995-82-0P
226995-84-2P 226995-85-3P 226995-86-4P 226995-87-5P 239077-04-4P
247256-15-1P 247256-16-2P 284031-00-1P 284031-06-7P 295780-86-8P
295793-48-5P 297132-09-3P 297132-10-6P 297132-11-7P
311339-03-4P 313505-06-5P 315678-22-9P 343600-10-2P 343945-05-1P
343965-02-6P 350690-08-3P 350690-10-7P 350690-11-8P 350690-12-9P
350690-14-1P 350690-15-2P 361364-46-7P 412339-45-8P 412340-49-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of phthalazines)

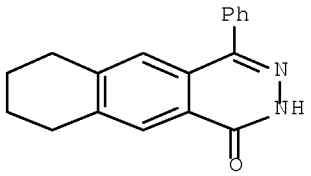
IT 295793-36-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phthalazines)

RN 295793-36-1 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-phenyl- (CA INDEX NAME)

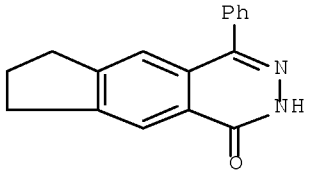


IT 173463-59-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of phthalazines)

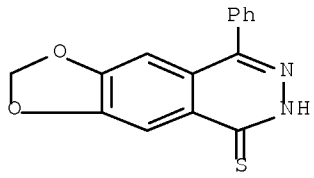
RN 173463-59-7 HCAPLUS
CN Benzo[g]phthalazin-1(2H)-one, 6,7,8,9-tetrahydro-4-phenyl- (CA INDEX NAME)



IT 173463-57-5P 295793-48-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of phthalazines)
RN 173463-57-5 HCAPLUS
CN 1H-Cyclopenta[g]phthalazin-1-one, 2,6,7,8-tetrahydro-4-phenyl- (CA INDEX NAME)



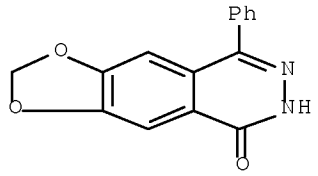
RN 295793-48-5 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazine-5(6H)-thione, 8-phenyl- (CA INDEX NAME)



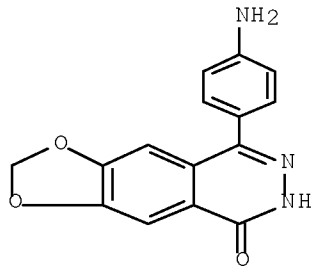
REFERENCE COUNT: 384 THERE ARE 384 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 11 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:928884 HCAPLUS Full-text
DOCUMENT NUMBER: 140:156731
TITLE: 1-Aryl-6,7-methylenedioxy-3H-quinazolin-4-ones as anticonvulsant agents
AUTHOR(S): Zappala, Maria; Grasso, Silvana; Micale, Nicola; Zuccala, Giuseppe; Menniti, Frank S.; Ferreri, Guido; De Sarro, Giovambattista; De Micheli, Carlo
CORPORATE SOURCE: Dipartimento Farmaco-Chimico, Universita di Messina, Messina, 98168, Italy
SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(24), 4427-4430
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:156731
ED Entered STN: 28 Nov 2003
AB A set of novel 1-aryl-6,7-methylenedioxy-3H-quinazolin-4-(thi)ones has been designed and screened as anticonvulsant agents in DBA/2 mice. The new compds. are provided with anticonvulsant properties comparable to those of GYKI 52466. To clarify the mode of action, their affinity for the quinazolinone/2,3-benzodiazepine site of the AMPA receptor complex has been assayed.
CC 1-3 (Pharmacology)
Section cross-reference(s): 27, 28
IT 253-52-1D, Phthalazine, derivs. 102771-26-6, GYKI 52466 197368-44-8 197368-47-1 197368-49-3 250699-43-5 295793-36-1 295793-40-7 295793-49-6 656833-90-8D, derivs. 656833-91-9D, derivs. 656834-00-3 656834-01-4 656834-02-5 656834-03-6 656834-04-7
RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
(arylmethylenedioxyquinazolinones as anticonvulsant agents)
IT 295793-36-1 295793-40-7 295793-49-6 656834-02-5 656834-03-6 656834-04-7
RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
(arylmethylenedioxyquinazolinones as anticonvulsant agents)
RN 295793-36-1 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-phenyl- (CA INDEX NAME)

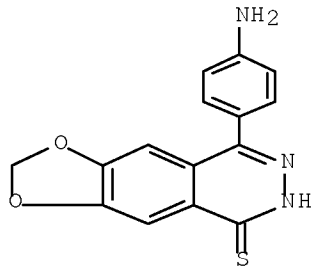


RN 295793-40-7 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-aminophenyl)- (CA INDEX NAME)

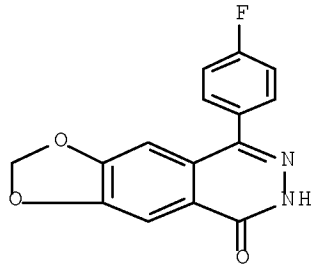


RN 295793-49-6 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazine-5(6H)-thione, 8-(4-aminophenyl)- (CA INDEX

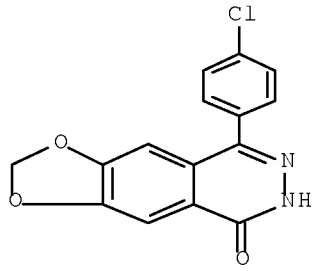
NAME)



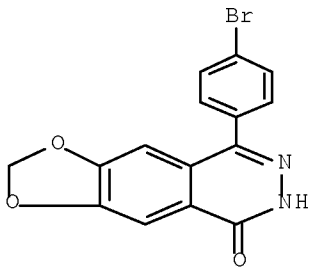
RN 656834-02-5 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-fluorophenyl)- (CA INDEX NAME)



RN 656834-03-6 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-chlorophenyl)- (CA INDEX NAME)

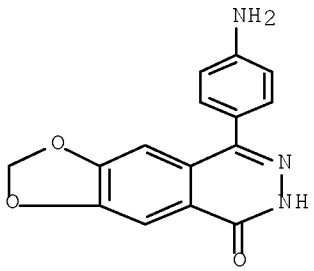


RN 656834-04-7 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-bromophenyl)- (CA INDEX NAME)

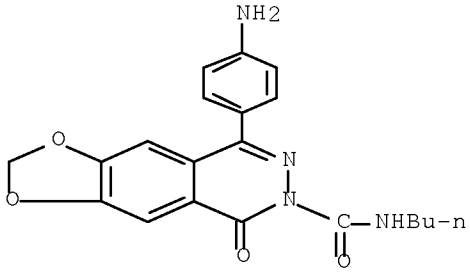


REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 12 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:91244 HCAPLUS Full-text
DOCUMENT NUMBER: 139:62588
TITLE: Characterization of the mechanism of anticonvulsant activity for a selected set of putative AMPA receptor antagonists
AUTHOR(S): Grasso, Silvana; Micale, Nicola; Zappala, Maria; Galli, Alessandro; Costagli, Chiara; Menniti, Frank S.; De Micheli, Carlo
CORPORATE SOURCE: Dipartimento Farmaco-Chimico, Universita di Messina, Messina, 98168, Italy
SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(3), 443-446
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 06 Feb 2003
AB A selected set of 1-aryl-7,8-methylenedioxy-2,3-benzodiazepin-4-ones and their analogs were evaluated for their ability to bind the competitive and noncompetitive sites of the AMPA receptors complex as well as to the glycine site of the NMDA receptors. The results put in evidence that most of the test compds., despite a close structural similarity with GYKI 52466, possess a significantly different pharmacol. profile.
CC 1-3 (Pharmacology)
IT 197368-49-3 197368-92-6 250699-34-4 295793-40-7 295793-45-2 343870-22-4 473451-53-5 473451-54-6 552290-38-7 552290-39-8 552290-40-1
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(mechanism of anticonvulsant activity for putative AMPA receptor antagonists)
IT 295793-40-7 295793-45-2
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(mechanism of anticonvulsant activity for putative AMPA receptor antagonists)
RN 295793-40-7 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-aminophenyl)- (CA INDEX NAME)



RN 295793-45-2 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide, 8-(4-aminophenyl)-N-butyl-5-oxo- (CA INDEX NAME)



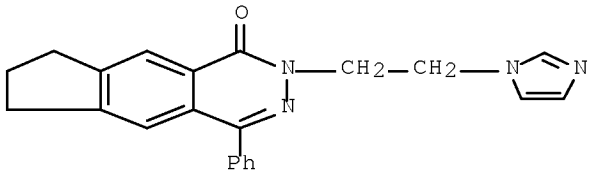
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 13 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:747676 HCAPLUS Full-text
DOCUMENT NUMBER: 132:30247
TITLE: Synthesis of 2-[2-(1-imidazolyl)ethyl]-4-phenylcycloalka[g]phthalazin-1(2H)-ones as thromboxane A2 synthase inhibitors
AUTHOR(S): Haider, Norbert; Hartmann, Rolf W.; Steinwender, Andreas
CORPORATE SOURCE: Institute Pharmaceutical Chemistry, Univ. Vienna, Vienna, A-1090, Austria
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1999), 332(11), 408-409
CODEN: ARPMAS; ISSN: 0365-6233
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 24 Nov 1999
AB A series of 2-[2-(1-imidazolyl)ethyl]-4-phenylcycloalka[g]phthalazin-1(2H)-ones with variable cycloalkene ring size was prepared and tested in vitro for thromboxane A2 synthase inhibitory activity.
CC 1-1 (Pharmacology)
IT 119-39-1P, Phthalazinone 137381-09-0P 252662-91-2P 252662-92-3P 252662-93-4P 252662-94-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

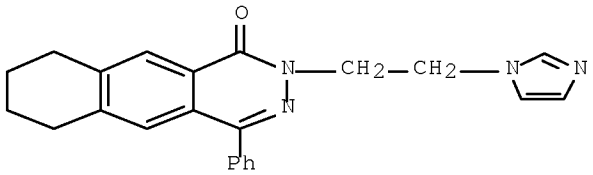
BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of 2-[2-(1-imidazolyl)ethyl]-4-phenylcycloalka[g]phthalazin-1(2H)-ones as thromboxane A2 synthase inhibitors)

IT 252662-91-2P 252662-92-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of 2-[2-(1-imidazolyl)ethyl]-4-phenylcycloalka[g]phthalazin-1(2H)-ones as thromboxane A2 synthase inhibitors)

RN 252662-91-2 HCAPLUS
CN 1H-Cyclopenta[g]phthalazin-1-one, 2,6,7,8-tetrahydro-2-[2-(1H-imidazol-1-yl)ethyl]-4-phenyl- (CA INDEX NAME)

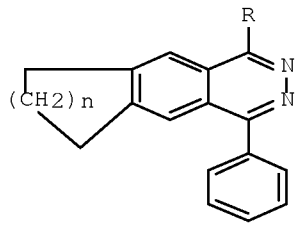


RN 252662-92-3 HCAPLUS
CN Benzo[g]phthalazin-1(2H)-one, 6,7,8,9-tetrahydro-2-[2-(1H-imidazol-1-yl)ethyl]-4-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 14 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:577161 HCAPLUS Full-text
DOCUMENT NUMBER: 125:300931
ORIGINAL REFERENCE NO.: 125:56327a,56330a
TITLE: Synthesis of g-annelated phthalazines as potential blood platelet aggregation inhibitors
AUTHOR(S): Haider, Norbert; Steinwender, Andreas
CORPORATE SOURCE: Institute Pharmaceutical Chemistry, University Vienna, Vienna, A-1090, Austria
SOURCE: Scientia Pharmaceutica (1996), 64(3/4), 399-405
CODEN: SCPHA4; ISSN: 0036-8709
PUBLISHER: Oesterreichische Apotheker-Verlagsgesellschaft
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 27 Sep 1996
GI



I

AB The phthalazines I (n = 1-4; R = NHR1; R1 = 3-ClC6H4, CH2CMe3) were prepared from the corresponding phthalazinones via the chloro compds. I (n = 1-4; R = Cl).

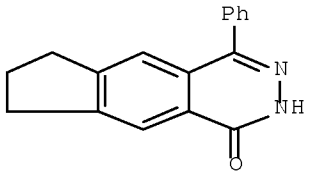
CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 108-42-9, 3-Chloroaniline 5813-64-9 173463-57-5 173463-59-7 173463-61-1 173463-63-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phthalazines)

IT 173463-57-5 173463-59-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phthalazines)

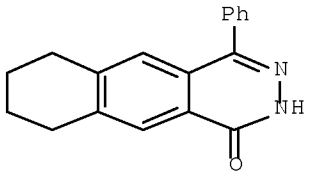
RN 173463-57-5 HCAPLUS

CN 1H-Cyclopenta[g]phthalazin-1-one, 2,6,7,8-tetrahydro-4-phenyl- (CA INDEX NAME)



RN 173463-59-7 HCAPLUS

CN Benzo[g]phthalazin-1(2H)-one, 6,7,8,9-tetrahydro-4-phenyl- (CA INDEX NAME)



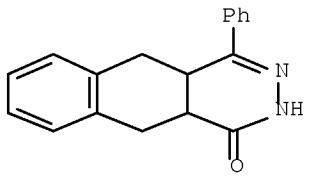
L55 ANSWER 15 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1958:87987 HCAPLUS Full-text

DOCUMENT NUMBER: 52:87987

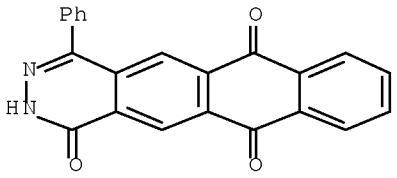
ORIGINAL REFERENCE NO.: 52:15487a-f
TITLE: Polycyclic compounds. IV. 2,9-Dimethyl-7,14-dioxo-5,12-dihydropentacene-6,13-quinone and 5,12-dihydrotetracene
AUTHOR(S): Buchta, Emil; Egger, Hermann
CORPORATE SOURCE: Univ. Erlangen, Germany
SOURCE: Chemische Berichte (1957), 90, 2760-3
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB cf. C.A. 51, 10466g. 2,5-Bis(2,5-dimethylbenzoyl)hydroquinone (I) (5 g.) heated to 340° and the sublimate recrystd. from 70% EtOH gave 900 mg. 2,5-Me2C6H3CO2H, needles, m. 132°. 2,5-Bis(2,5-dimethylbenzoyl)-p-quinone (6 g.) and 3 g. glass powder heated to 380°, kept 30-40 min. at this temperature, cooled, powdered, and sublimed at 0.4 mm. gave to 250° I and from 350-60° a glassy red product which extracted twice with Et2O and recrystd. from xylene gave 2,9-dimethyl-7,14-dioxo-5,12-dihydropentacene-6,13-quinone, light brown needles, m. 384-6°; it gave a blue solution with intense red fluorescence in concentrated H2O4. o-C6H4(CH2Br)2 (52 g.) in 250 cc. absolute EtOH, 63 g. [CH(CO2Et)2]2 in 300 cc. absolute EtOH, and 9.5 g. Na in 140 cc. EtOH heated 6 hrs. in an autoclave to 130° and concentrated, the residue dissolved in a little H2O, acidified with dilute H2SO4, and extracted with Et2O, and the extract worked up gave 70 g. tetra-Et 1,2,3,4-tetrahydronaphthalene-2,2,3,3-tetracarboxylate (II), viscous oil, b0.01 170°. II (42 g.) in 60 cc. MeOH refluxed with 100 cc. 40% KOH in MeOH, the MeOH distilled, the residue dissolved in 150 cc. H2O, the solution filtered, acidified with 2N H2SO4, and extracted with Et2O, the extract dried and evaporated, and the oily residue heated to 180-90° until the CO2 and H2O elimination ceased, cooled, and triturated with Et2O gave 14g. 1,2,3,4-tetrahydronaphthalene-2,3-dicarboxylic acid anhydride (III), m. 184°. III (5 g.) in 150 cc. dry C6H6 treated with 6.7 g. powdered AlCl3, refluxed 2 hrs., poured into ice and concentrated HCl, and filtered yielded 6.5 g. 2-benzoyl-1,2,3,4-tetrahydronaphthalene-3-carboxylic acid (IV), m. 182-4° (xylene). IV (2 g.) in 20 cc. 92% N2H4.H2O refluxed 1 hr. and cooled gave 1.5 g. 1-phenyl-4-hydroxy-4a,9,9a,10-tetrahydro-2,3-diazaanthracene, m. 198° (98% EtOH). Zn dust (30 g.), 3 g. HgCl2 in 150 cc. H2O, and 5 cc. concentrated HCl shaken 5 min., the solution decanted, the residue refluxed 24 hrs. with 20 cc. H2O and 45 cc. concentrated HCl, 10 g. IV, 150 cc. PhMe, and 3 cc. glacial AcOH while adding at 6 hr.-intervals 20-cc. portions of concentrated HCl and cooled, and the PhMe layer evaporated yielded 8.6 g. 2-PhCH2 analog (V) of IV, m. 146-8° (50% AcOH). V (2 g.) and 3 g. NaCl heated under a stream of N at 310° until the elimination of H2O ceased, cooled, dissolved in dilute HCl, and filtered, and the residue triturated with Et2O gave 1 g. 5,12-dihydrotetracene, needles, m. 208-9° (xylene).
CC 10 (Organic Chemistry)
IT 610-72-0P, Benzoic acid, 2,5-dimethyl- 959-02-4P, Naphthacene, 5,12-dihydro- 29811-05-0P, 2,3-Naphthalenedicarboxylic anhydride, 1,2,3,4-tetrahydro- 76044-99-0P, 2,2,3,3-Naphthalenetetracarboxylic acid, 1,4-dihydro-, tetraethyl ester 101723-54-0P, 2-Naphthoic acid, 3-benzoyl-1,2,3,4-tetrahydro- 101789-59-7P, 2-Naphthoic acid, 3-benzyl-1,2,3,4-tetrahydro- 109892-05-9P, Benzo[g]phthalazin-1-ol, 4a,5,10,10a-tetrahydro-4-phenyl- 114722-26-8P, 5,6,12,13(7H,14H)-Pentacenetetrone, 3,10-dimethyl-
RL: PREP (Preparation)
(preparation of)
IT 109892-05-9P, Benzo[g]phthalazin-1-ol, 4a,5,10,10a-tetrahydro-4-phenyl-
RL: PREP (Preparation)
(preparation of)

RN 109892-05-9 HCAPLUS
CN Benzo[g]phthalazin-1(2H)-one, 4a,5,10,10a-tetrahydro-4-phenyl- (CA INDEX NAME)



L55 ANSWER 16 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1931:16478 HCAPLUS Full-text
DOCUMENT NUMBER: 25:16478
ORIGINAL REFERENCE NO.: 25:1821h-i,1822a
TITLE: Pyromellitic acid. Benzodiketohydrindene and benzodipyridazine derivatives
AUTHOR(S): Seka, Reinhard; Sedlatschek, Hans; Preissecker, Heinrich
SOURCE: Monatshefte fuer Chemie (1931), 57, 86-96
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 16 Dec 2001
AB O(CO)2C6H2(CO)2O (I) and quinaldine, heated at 250° until the mass is solid, give the condensation product (II), C30H16O4N2, dark reddish brown, decomps. 265°, insol. in EtOH, and the yellow-brown, EtOH-soluble compound, C20H11O6N, decomps. about 125°. Sulfonation of II with 50% oleum at 170° gives a product similar to quinoline yellow, which dyes wool and silk a pure yellow. I and α-C10H7NH2 give pyromellitic dinaphthylimide, m. 431°. N2H4.H2O (4 mols.) gives the dihydrazide, light yellow, decomps. about 450°; its tetra-Ac derivative m. 235-8°. 1,4,2,5-Bz2C6H2(CO2H)2 and 10 mols. N2H4.H2O in absolute EtOH, heated 24 hrs. at 120°, give 90% of 1,6-diphenyl-4,9-dihydroxybenzodipyridazine, carbonizes at 445°; 1,5,2,4-Bz2C6H2(CO2H)2 and 6 mols. N2H4.H2O give the 1,9-diphenyl-4,6-dihydroxy derivative, decomps. 430°. (MeC5H4CO)2C6H2(CO2H)2 and N2H4.H2O give the 1,9-dixylyl-4,6-dihydroxy derivative, carbonizes at a high temperature 2-Benzoylanthraquinone-3-carboxylic acid and 3.8 mols. N2H4.H2O in absolute EtOH, heated 9 hrs. at 120°, give the hydrazide, light yellow, decomps. 374°. 1,2,4,5-C6H2(COCl)4 and MeONa in C6H6 give 88% of tetra-Me pyromellitate, m. 138°; the tetra-Ph ester, m. 179.5°, results in 24% yields.
CC 10 (Organic Chemistry)
IT 4760-87-6P, Pyridazo[4,5-g]phthalazine-1,4,6,9(2,3,7,8)-tetrone
31663-83-9P, Pyromellitimide, N,N'-di-1-naphthyl- 161535-66-6P, Pyridazo[4,5-g]phthalazine-1,6-diol, 4,9-diphenyl- 161535-67-7P, Pyridazo[4,5-g]phthalazine-1,9-diol, 4,6-diphenyl- 853118-02-2P, Pyridazo[4,5-g]phthalazine-1,4,6,9(2,3,7,8)-tetrone, 2,3,7,8-tetraacetyl- 858020-38-9P, Naphtho[2,3-g]phthalazine-6,11-dione, 1-hydroxy-4-phenyl-
RL: PREP (Preparation)
(preparation of)
IT 858020-38-9P, Naphtho[2,3-g]phthalazine-6,11-dione, 1-hydroxy-4-phenyl-
RL: PREP (Preparation)
(preparation of)

RN 858020-38-9 HCAPLUS
CN Naphtho[2,3-g]phthalazine-1,6,11(2H)-trione, 4-phenyl- (CA INDEX NAME)

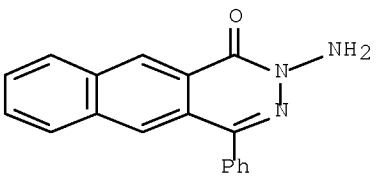


=> d 17
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CAOLD, CHEMCATS, CHEMINFORMRX' -
CONTINUE? (Y)/N:y

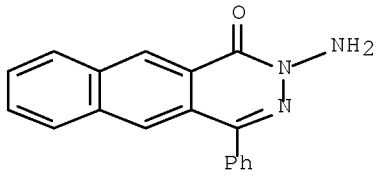
L55 ANSWER 17 OF 24 CAOLD COPYRIGHT 2008 ACS on STN
AN CA52:15486i CAOLD
TI unsatd. hydrocarbons
AU Kotlyarevskii, I. L.; Zanina, A. S.; Lipovich, V. G.
IT 959-02-4 1076-61-5 1559-81-5 1680-51-9 2809-64-5
3877-19-8 21564-92-1 29811-05-0 76044-99-0 101723-54-0 101789-59-7
109892-05-9 114722-26-8

=> d ide 18-20
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CAOLD, CHEMCATS, CHEMINFORMRX' -
CONTINUE? (Y)/N:y

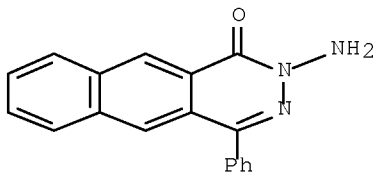
L55 ANSWER 18 OF 24 CHEMCATS COPYRIGHT 2008 ACS on STN
Accession No. (AN): 2043513538 CHEMCATS
Catalog Name (CO): Ryan Scientific Screening Library
Publication Date (PD): 25 Jan 2008
Order Number (ON): AK-830/13217101
Chemical Name (CN): Benzo[g]phthalazin-1(2H)-one, 2-amino-4-phenyl-
CAS Registry No. (RN): 445224-50-0
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



L55 ANSWER 19 OF 24 CHEMCATS COPYRIGHT 2008 ACS on STN
Accession No. (AN): 2020466079 CHEMCATS
Catalog Name (CO): Interchim Intermediates
Publication Date (PD): 18 Feb 2008
Order Number (ON): AK-830/13217101
Chemical Name (CN): Benzo[g]phthalazin-1(2H)-one, 2-amino-4-phenyl-
CAS Registry No. (RN): 445224-50-0
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



L55 ANSWER 20 OF 24 CHEMCATS COPYRIGHT 2008 ACS on STN
Accession No. (AN): 2017061712 CHEMCATS
Catalog Name (CO): Compounds For Screening
Publication Date (PD): 2 Oct 2008
Order Number (ON): AK-830/13217101
Chemical Name (CN): 2-amino-4-phenylbenzo[g]phthalazin-1(2H)-one
CAS Registry No. (RN): 445224-50-0
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :

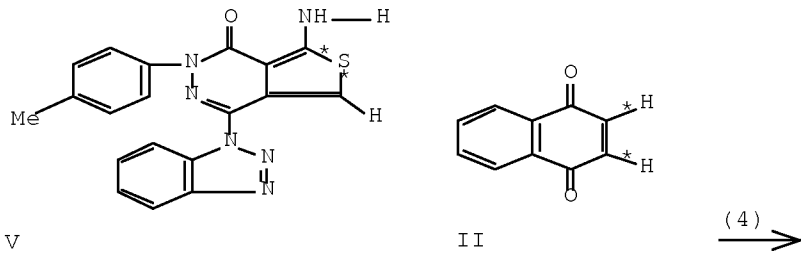


=> d bib ab hit 21-24
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CAOLD, CHEMCATS, CHEMINFORMRX' -
CONTINUE? (Y)/N:y

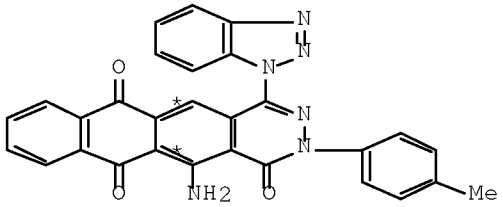
L55 ANSWER 21 OF 24 CHEMINFORMRX COPYRIGHT 2008 FIZ CHEMIE on STN

AN 200534151 CHEMINFORMRX Full-text
TI Studies with Condensed Thiophenes: Reactivity of Condensed Aminothiophenes Toward Carbon and Nitrogen Electrophiles.
AU AL-SALEH, B.; ABDELKHALIK, M. M.; EL-APASERY, M. A.; ELNAGDI, M. H.
CS Dep. Chem., Fac. Sci., Univ. Kuwait, Safat 13060, Kuwait
SO J. Chem. Res.(1), 23-26 (2005)
CODEN: JCROA4 ISSN: 0308-2342
LA English

RX(4) OF 17 I + B ===> J



V II (4)

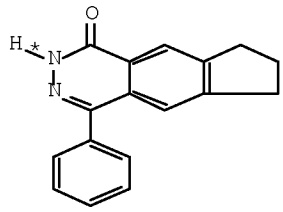


VI
YIELD 56.0%

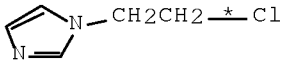
RX(4) RCT V, 727009
II, 1180 (130-15-4)
SOL 81 (64-17-5), EtOH
PRO VI, 1097121
YDS 56.0 %
T.KW REFLUX
KW aromatisation; alkylation; C-alkylation
NTE reaction:V (II) -> VI, example: 2

L55 ANSWER 22 OF 24 CHEMINFORMRX COPYRIGHT 2008 FIZ CHEMIE on STN
AN 200007133 CHEMINFORMRX Full-text
TI Synthesis of 2-[2-(1-Imidazolyl)ethyl]-4-phenylcycloalka[g]phthalazin-1(2H)-ones as Thromboxane A2 Synthase Inhibitors.
AU HAIDER, N.; HARTMANN, R. W.; STEINWENDER, A.
CS Inst. Pharm. Chem., Univ. Wien, A-1090 Wien, Austria
SO Arch. Pharm. (Weinheim, Ger.), 332(11), 408-409 (1999)
CODEN: ARPMAS ISSN: 0365-6233
LA English
AB The title compounds (III) show thromboxane A2 synthase inhibitory activity which decreases with increasing ring size.

RX(1) OF 3 A + B ===> C

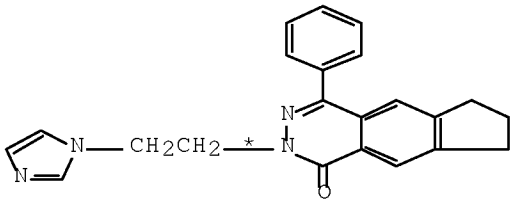


I



II

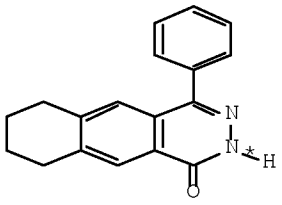
(1) →



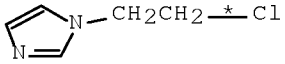
III
YIELD 68.0%

RX(1) RCT I, 447880
II, 720168
RGT 1163 (7646-69-7), NaH
SOL 76 (68-12-2), DMF
PRO III, 720169
YDS 68.0 %
T 25.0 - 70.0 Cel
KW alkylation; N-alkylation
NTE reaction:I (II) -> III, example: 1

RX(2) OF 3 F + B ===> G

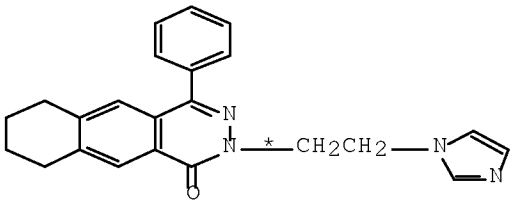


I



II

(2) →

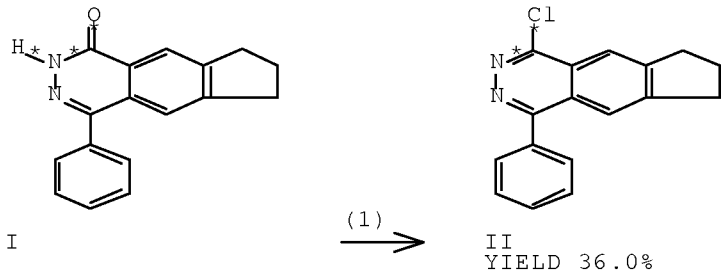


III
YIELD 70.0%

RX(2) RCT I, 527603
II, 720168
RGT 1163 (7646-69-7), NaH
SOL 76 (68-12-2), DMF
PRO III, 720170
YDS 70.0 %
T 25.0 - 70.0 Cel
KW alkylation; N-alkylation
NTE reaction:I (II) -> III, example: 2

L55 ANSWER 23 OF 24 CHEMINFORMRX COPYRIGHT 2008 FIZ CHEMIE on STN
AN 199718188 CHEMINFORMRX Full-text
TI Synthesis of g-Annelated Phthalazines as Potential Blood Platelet Aggregation Inhibitors.
AU HAIDER, N.; STEINWENDER, A.
CS Inst. Pharm. Chem., Univ. Wien, A-1090 Wien, Austria
SO Sci. Pharm., 64(3), 399-405 (1996)
CODEN: SCPHA4 ISSN: 0036-8709
LA English
AB A series of cycloalkene-fused 1-arylamino- and 1-alkylamino-4-phenylphthalazines (IV) (8 examples) is prepared by amination of readily achieved chloro compounds (II). Compounds (IV) represent a novel type of analogues of known antiaggregatory agents, however, only compound (IIIa) exhibits some platelet antiaggregatory potency.

RX(1) OF 11 A ===> B...

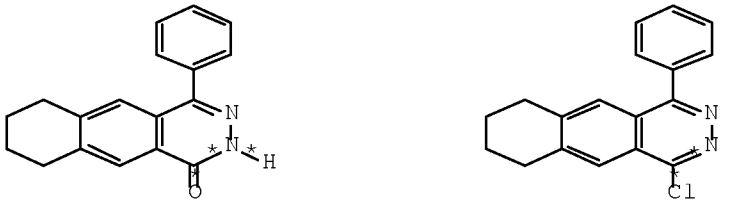


I II
YIELD 36.0%

RX(1) RCT I, 447880
RGT 181 (10025-87-3), POCl3
63 (91-66-7), Ph-NEt2
PRO II, 527602
YDS 36.0 %
T 90.0 Cel

KW aromatisation; halogenation; C-halogenation; chlorination; alkylation
NTE reaction:I -> II, example: 1

RX(2) OF 11 E ===> F...

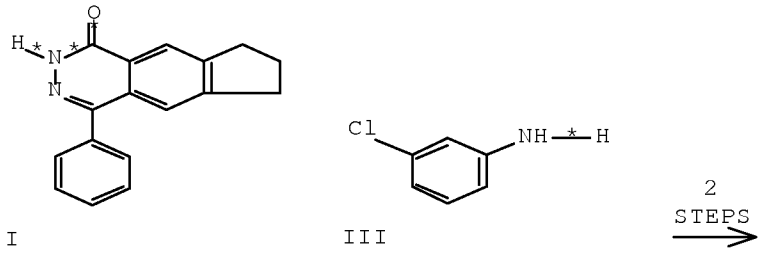


I

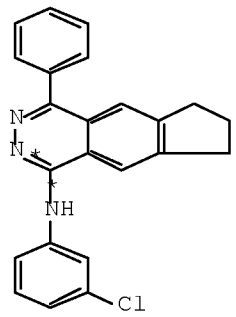
II
YIELD 50.0%

RX(2) RCT I, 527603
RGT 181 (10025-87-3), POCl3
63 (91-66-7), Ph-NEt2
PRO II, 527604
YDS 50.0 %
T 90.0 Cel
KW aromatisation; halogenation; C-halogenation; chlorination; alkylation
NTE reaction:I -> II, example: 2

RX(8) OF 11 COMPOSED OF RX(1), RX(4)
RX(8) A + I ===> J



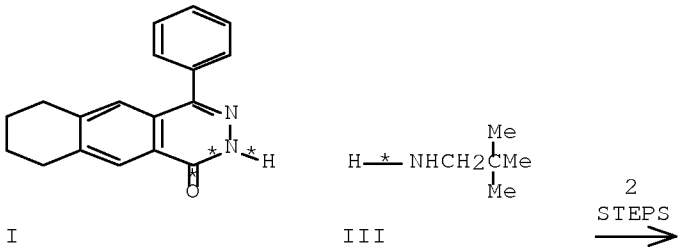
I III



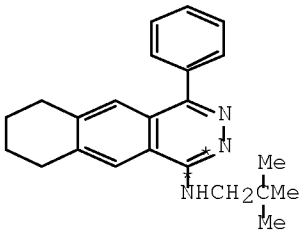
IV

RX(1) RCT I, 447880
RGT 181 (10025-87-3), POCl3
63 (91-66-7), Ph-NEt2
PRO II, 527602
YDS 36.0 %
T 90.0 Cel
KW aromatisation; halogenation; C-halogenation; chlorination; alkylation
NTE reaction:I -> II, example: 1
RX(4) RCT II, 527602
III, 14699 (108-42-9)
SOL 80 (123-91-1), dioxane
PRO IV, 527606
T 130.0 Cel
KW arylation
NTE [sealed tube]; reaction:II (III) -> IV, example: 1

RX(9) OF 11 COMPOSED OF RX(2), RX(5)
RX(9) E + L ===> M



I III



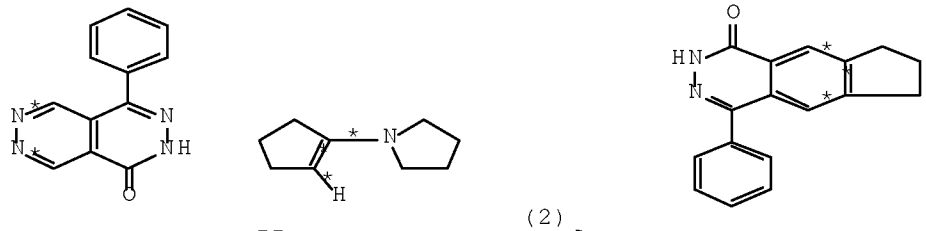
IV

RX(2) RCT I, 527603
RGT 181 (10025-87-3), POCl3
63 (91-66-7), Ph-NEt2
PRO II, 527604
YDS 50.0 %
T 90.0 Cel
KW aromatisation; halogenation; C-halogenation; chlorination; alkylation
NTE reaction:I -> II, example: 2
RX(5) RCT II, 527604
III, 370369

SOL 80 (123-91-1), dioxane
PRO IV, 527607
T 100.0 Cel
KW arylation
NTE [sealed tube]; reaction:II (III) -> IV, example: 2

L55 ANSWER 24 OF 24 CHEMINFORMRX COPYRIGHT 2008 FIZ CHEMIE on STN
AN 199612174 CHEMINFORMRX Full-text
TI Inverse-Electron-Demand Diels-Alder Reactions of Condensed Pyridazines. Part 8. Convenient Synthesis of Cycloalkene-Fused Phthalazinones.
AU HAIDER, N.
CS Inst. Pharm. Chem., Univ. Wien, A-1090 Wien, Austria
SO Heterocycles, 41(11), 2519-2525 (1995)
CODEN: HTCYAM ISSN: 0385-5414
LA English
AB Cycloalkene-anellated phthalazin-1(2H)-ones (III) are easily prepared by an inverse-electron-demand Diels-Alder reaction of the pyridazinopyridazine (I) with the enamines (II) followed by acid- catalyzed aromatization of intermediates (IV). C4-Substituted phthalazinones are key compounds in the synthesis of platelet aggregation or thromboxane A2 synthetase inhibitors.

RX(2) OF 4 G + B ===> H



RX(2) RCT I, 447879
II, 17585 (7148-07-4)
STAGE(1)
SOL 80 (123-91-1), dioxane
T.KW REFLUX
TIM 1.0 hr
STAGE(2)
RGT 3 (64-19-7), AcOH
SOL 182 (71-23-8), PrOH
T.KW REFLUX
TIM 24 hr
PRO III, 447880
YDS 84.0 %
KW aromatisation; addition; olefination
NTE reaction:I + II -> III, example: 2
CMT #E0100:(100% e.e.|92% d.e.)

```
=> fil beilst
FILE 'BEILSTEIN' ENTERED AT 15:50:54 ON 04 DEC 2008
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FILE LAST UPDATED ON April 1, 2008

FILE COVERS 1771 TO 2008.
*** FILE CONTAINS 10.322,808  SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in
   separate documents and can not be searched together in one query.
   Reaction data for BEILSTEIN compounds may be displayed
   immediately with the display codes PRE (preparations) and REA
   (reactions).  A substance answer set retrieved after the search
   for a chemical name, a compounds with available reaction
   information by combining with PRE/FA, REA/FA or more generally
   with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
   between a BEILSTEIN compound and belonging reactions. For mo
   detailed reaction searches BRNs can be searched as reaction
   partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE  <<<

**********************************************************************
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.                *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE   *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE          *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                        *
* FOR PRICE INFORMATION SEE HELP COST                                *
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>>> Price change as of January 1st, 2008: Connect Time and Structure
    Search fees re-introduced. See NEWS and HELP COST <<<

=> d que stat l39
L13             STR
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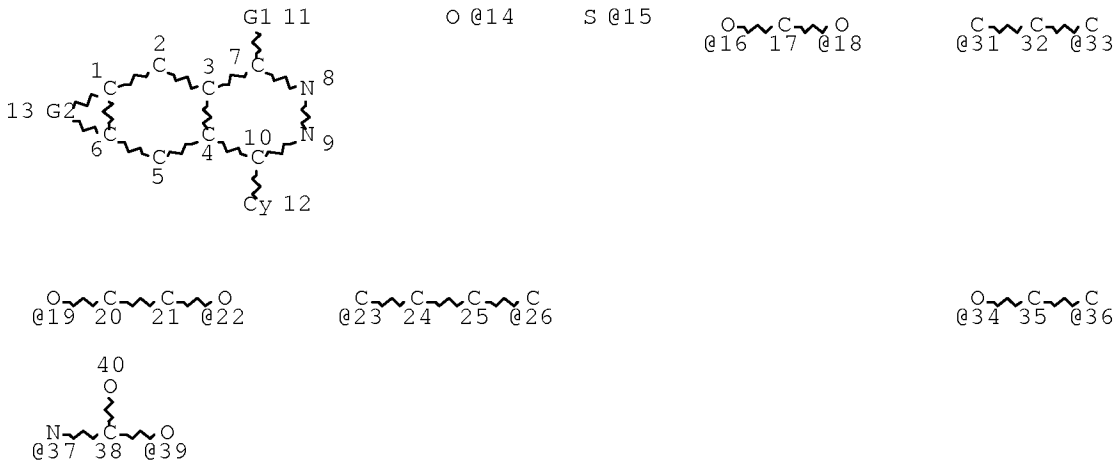


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9-1/39-6 37-1
NODE ATTRIBUTES:
CONNECT IS E1  RC AT  14
CONNECT IS E1  RC AT  15
CONNECT IS E1  RC AT  40
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT  12
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  36

STEREO ATTRIBUTES: NONE
L39          33 SEA FILE=BEILSTEIN SSS FUL L13

100.0% PROCESSED    3620 ITERATIONS                          33 ANSWERS
SEARCH TIME: 00.00.05
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```
=> d ide l39 1

L39  ANSWER 1 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

     Beilstein Records (BRN):        11079041
     Chemical Name (CN):             1,1'-bi(5'',6'',7,7'',8,8'',9,10-octahydro
                                     -5'',5'',7,7,8'',8''10,10-octamethyl-5,12-
                                     <2'',3''>naphthaleno-2,3-diazatetracenyl)-
                                     4,4'(3H,3'H)-dione
     Molec. Formula (MF):            C68 H78 N4 O2
     Molecular Weight (MW):          983.39
     Lawson Number (LN):             30560
     Compound Type (CTYPE):          heterocyclic
     Constitution ID (CONSID):       9259960
     Tautomer ID (TAUTID):           10315765
     Entry Date (DED):               2008/04/19
     Update Date (DUPD):             2008/04/19
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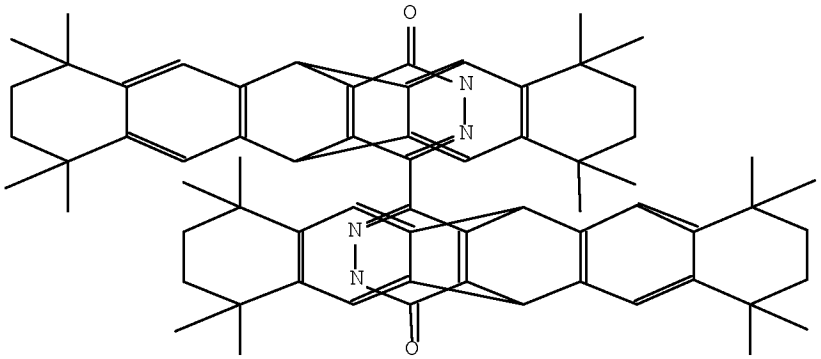

Field Availability:

Code	Name	Occurrence
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CN	Chemical Name	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
NMR	Nuclear Magnetic Resonance	4

This substance also occurs in Reaction Documents:

Code	Name	Occurrence

```
     ==========================================================
     RX        Reaction Documents                          2
     RXREA     Substance is Reaction Reactant              1
     RXPRO     Substance is Reaction Product               1


=> d rx l39 1


L39  ANSWER 1 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX
     Reaction ID (.ID):              10780544
     Reactant BRN (.RBRN):           11078905
     Reactant (.RCT):                1,1'-bi(5'',6'',7,7'',8,8'',9,10-octahydro
                                     -5'',5'',7,7,8'',8'',10,10-octamethyl-4-me
                                     thoxy-5,12-<2'',3''>naphthaleno-2,3-diazat
                                     etracenyl)
     Product BRN (.PBRN):            11079041
     Product (.PRO):                 1,1'-bi(5'',6'',7,7'',8,8'',9,10-octahydro
                                     -5'',5'',7,7,8'',8''10,10-octamethyl-5,12-
                                     <2'',3''>naphthaleno-2,3-diazatetracenyl)-
                                     4,4'(3H,3'H)-dione
     No. of React. Details (.NVAR):  1

Reaction Details:
RX
     Reaction RID (.RID):            10780544.1
     Reaction Classification (.CL):  Preparation
     Yield (.YDT):                   100 percent (BRN=11079041)
     Reagent (.RGT):                 HBr, AcOH
     Temperature (.T):               95 Cel
     Reference(s):
     1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M.,
        J. Org. Chem., CODEN: JOCEAH, SIR72(26), <2007>, 10166 - 10180;
        BABS-6716975

Reaction:
RX
     Reaction ID (.ID):              10780576
     Reactant BRN (.RBRN):           11079041
     Reactant (.RCT):                1,1'-bi(5'',6'',7,7'',8,8'',9,10-octahydro
                                     -5'',5'',7,7,8'',8''10,10-octamethyl-5,12-
                                     <2'',3''>naphthaleno-2,3-diazatetracenyl)-
                                     4,4'(3H,3'H)-dione
     Product BRN (.PBRN):            11078937
     Product (.PRO):                 1,1'-bi(4-chloro-5'',6'',7,7'',8,8'',9,10-
                                     octahydro-5'',5'',7,7,8'',8'',10,10-octame
                                     thyl-5,12-<2'',3''>naphthaleno-2,3-diazate
                                     tracenyl)
     No. of React. Details (.NVAR):  1

Reaction Details:
RX
     Reaction RID (.RID):            10780576.1
     Reaction Classification (.CL):  Preparation
     Yield (.YDT):                   79 percent (BRN=11078937)
     Reagent (.RGT):                 POCl3
     Temperature (.T):               80 Cel
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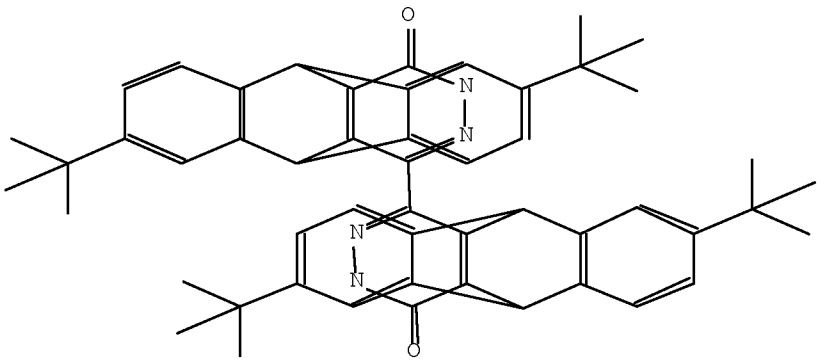
Reference(s):
1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M., J. Org. Chem., CODEN: JOCEAH, SIR72(26), <2007>, 10166 - 10180; BABS-6716975

=> d ide l39 2

L39 ANSWER 2 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	11074617
Chemical Name (CN):	1,1'-bi(5'',6-di-tert-butyl-9,10-dihydro-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl)-4,4'(3H,3'H)-dione
Molec. Formula (MF):	C52 H54 N4 O2
Molecular Weight (MW):	767.02
Lawson Number (LN):	30564
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	9256297
Tautomer ID (TAUTID):	10313539
Entry Date (DED):	2008/04/19
Update Date (DUPD):	2008/04/19



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1

NMR	Nuclear Magnetic Resonance	6

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 2

L39 ANSWER 2 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	10779415
Reactant BRN (.RBRN):	11074651
Reactant (.RCT):	1,1'-bi(5'',6-di-tert-butyl-9,10-dihydro-4-methoxy-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl)
Product BRN (.PBRN):	11074617
Product (.PRO):	1,1'-bi(5'',6-di-tert-butyl-9,10-dihydro-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl)-4,4'(3H,3'H)-dione
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	10779415.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	97 percent (BRN=11074617)
Reagent (.RGT):	HBr, AcOH
Temperature (.T):	95 Cel

Reference(s):
1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M., J. Org. Chem., CODEN: JOCEAH, SIR72(26), <2007>, 10166 - 10180; BABS-6716975

Reaction:
RX

Reaction ID (.ID):	10779407
Reactant BRN (.RBRN):	11074617
Reactant (.RCT):	1,1'-bi(5'',6-di-tert-butyl-9,10-dihydro-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl)-4,4'(3H,3'H)-dione
Product BRN (.PBRN):	11074271
Product (.PRO):	1,1'-bi(5'',6-di-tert-butyl-4-chloro-9,10-dihydro-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl)
No. of React. Details (.NVAR):	1

Reaction Details:
RX

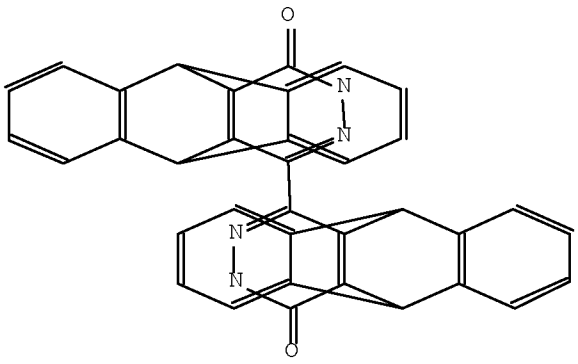
Reaction RID (.RID):	10779407.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	76 percent (BRN=11074271)
Reagent (.RGT):	POCl3

Temperature (.T): 60 Cel
Reference(s):
1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M., J. Org. Chem., CODEN: JOCEAH, SIR72(26), <2007>, 10166 - 10180; BABS-6716975

=> d ide l39 3

L39 ANSWER 3 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 11065936
Chemical Name (CN): 1,1'-bi(9,10-dihydro-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl)-4,4'(3H,3'H)-dione
Molec. Formula (MF): C36 H22 N4 O2
Molecular Weight (MW): 542.60
Lawson Number (LN): 30560
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 9249543
Tautomer ID (TAUTID): 10311733
Entry Date (DED): 2008/04/19
Update Date (DUPD): 2008/04/19



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1

NMR	Nuclear Magnetic Resonance	4

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3
RXREA	Substance is Reaction Reactant	2
RXPRO	Substance is Reaction Product	1

=> d rx l39 3

L39 ANSWER 3 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	10776880
Reactant BRN (.RBRN):	11065310
Reactant (.RCT):	1,1'-bi(9,10-dihydro-4-methoxy-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl)
Product BRN (.PBRN):	11065936
Product (.PRO):	1,1'-bi(9,10-dihydro-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl)-4,4'(3H,3'H)-dione
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	10776880.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	91 percent (BRN=11065936)
Reagent (.RGT):	HBr, AcOH
Temperature (.T):	90 Cel

Reference(s):
1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M., J. Org. Chem., CODEN: JOCEAH, SIR72(26), <2007>, 10166 - 10180; BABS-6716975

Reaction:
RX

Reaction ID (.ID):	10777066
Reactant BRN (.RBRN):	11065936
Reactant (.RCT):	1,1'-bi(9,10-dihydro-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl)-4,4'(3H,3'H)-dione
Product BRN (.PBRN):	11065026
Product (.PRO):	1,1'-bi(4-bromo-9,10-dihydro-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl)
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	10777066.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	39 percent (BRN=11065026)
Reagent (.RGT):	POBr3
Solvent (.SOL):	toluene
Temperature (.T):	90 Cel

Reference(s):
1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M.,

J. Org. Chem., CODEN: JOCEAH, SIR72(26), <2007>, 10166 - 10180; BABS-6716975

Reaction:
RX

Reaction ID (.ID):	10777065
Reactant BRN (.RBRN):	11065936
Reactant (.RCT):	1,1'-bi(9,10-dihydro-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl)-4,4'(3H,3'H)-dione
Product BRN (.PBRN):	11064586
Product (.PRO):	1,1'-bi(4-chloro-9,10-dihydro-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl)
No. of React. Details (.NVAR):	1

Reaction Details:
RX

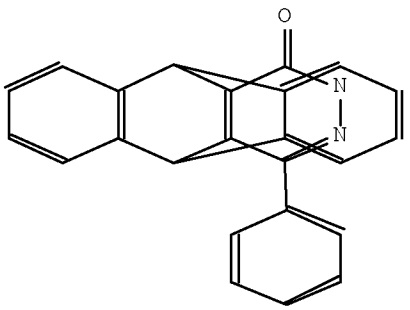
Reaction RID (.RID):	10777065.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	66 percent (BRN=11064586)
Reagent (.RGT):	POCl3
Temperature (.T):	90 Cel

Reference(s):
1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M., J. Org. Chem., CODEN: JOCEAH, SIR72(26), <2007>, 10166 - 10180; BABS-6716975

=> d ide l39 4

L39 ANSWER 4 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	11028913
Chemical Name (CN):	9,10-dihydro-4-phenyl-9,10-<1',2'>benzeno-2,3-diazaanthracen-1(2H)-one
Molec. Formula (MF):	C24 H16 N2 O
Molecular Weight (MW):	348.40
Lawson Number (LN):	28763
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	9218605
Tautomer ID (TAUTID):	10299045
Entry Date (DED):	2008/04/19
Update Date (DUPD):	2008/04/19



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
NMR	Nuclear Magnetic Resonance	4

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 4

L39 ANSWER 4 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	10767049
Reactant BRN (.RBRN):	11028325
Reactant (.RCT):	9,10-dihydro-1-methoxy-4-phenyl-9,10-<1',2'>benzeno-2,3-diazaanthracene
Product BRN (.PBRN):	11028913
Product (.PRO):	9,10-dihydro-4-phenyl-9,10-<1',2'>benzeno-2,3-diazaanthracen-1(2H)-one
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	10767049.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	72 percent (BRN=11028913)
Reagent (.RGT):	HBr, AcOH
Temperature (.T):	90 Cel

Reference(s):
1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M., J. Org. Chem., CODEN: JOCEAH, SIR72(26), <2007>, 10166 - 10180; BABS-6716975

Reaction:
RX

Reaction ID (.ID):	10767216
Reactant BRN (.RBRN):	11028913
Reactant (.RCT):	9,10-dihydro-4-phenyl-9,10-<1',2'>benzeno-

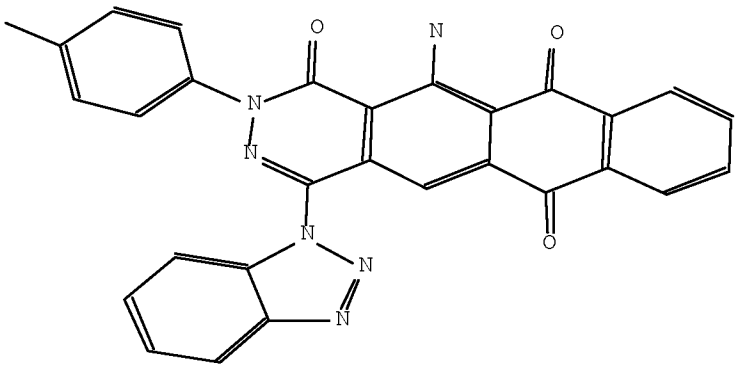
2,3-diazaanthracen-1(2H)-one
Product BRN (.PBRN): 11029222
Product (.PRO): 1-chloro-9,10-dihydro-4-phenyl-9,10-<1',2'>benzeno-2,3-diazaanthracene
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 10767216.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 90 percent (BRN=11029222)
Reagent (.RGT): POCl3
Other Conditions (.COND): Heating
Reference(s):
1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M., J. Org. Chem., CODEN: JOCEAH, SIR72(26), <2007>, 10166 - 10180; BABS-6716975

=> d ide l39 5

L39 ANSWER 5 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 9968931
Chemical Name (CN): 12-amino-4-benzotriazol-1-yl-2-p-tolyl-2H-2,3-diazanaphthacene-1,6,11-trione
Autonom Name (AUN): 12-amino-4-benzotriazol-1-yl-2-p-tolyl-2H-2,3-diaza-naphthacene-1,6,11-trione
Molec. Formula (MF): C29 H18 N6 O3
Molecular Weight (MW): 498.50
Lawson Number (LN): 30004, 29939, 16445
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 8391057
Tautomer ID (TAUTID): 9323912
Entry Date (DED): 2005/07/22
Update Date (DUPD): 2005/07/22



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
CPD	Crystal Property Description	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 5

L39 ANSWER 5 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	9815714
Reactant BRN (.RBRN):	8507609, 878524
Reactant (.RCT):	7-amino-4-benzotriazol-1-yl-2-p-tolyl-2H-thieno<3,4-d>pyridazin-1-one, <1,4>naphthoquinone
Product BRN (.PBRN):	9968931
Product (.PRO):	12-amino-4-benzotriazol-1-yl-2-p-tolyl-2H-2,3-diaza-naphthacene-1,6,11-trione
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	9815714.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	56 percent (BRN=9968931)
Solvent (.SOL):	ethanol
Time (.TIM):	10 hour(s)
Other Conditions (.COND):	Heating

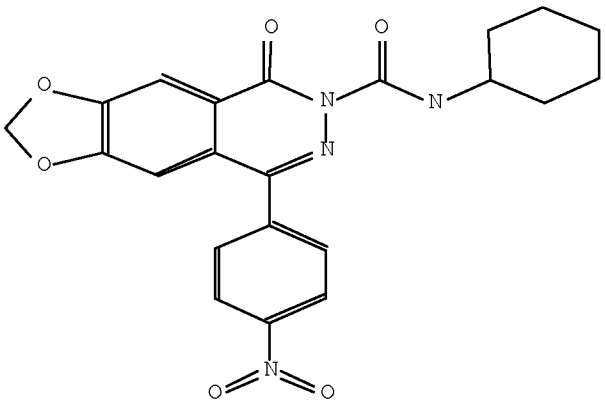
Reference(s):

1. Al-Saleh, Balkis; Abdelkhalik, Mervat M.; El-Apasery, Morsy A.; Elnagdi, Mohamed H., J. Chem. Res. Synop., CODEN: JRPSDC(1), <2005>, 23 - 26; BABS-6487077

=> d ide l39 6

L39 ANSWER 6 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	8806911
Chemical Name (CN):	8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid cyclohexylamide
Autonom Name (AUN):	8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid cyclohexylamide
Molec. Formula (MF):	C22 H20 N4 O6
Molecular Weight (MW):	436.42
Lawson Number (LN):	32359, 14011, 1762
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7455547
Tautomer ID (TAUTID):	8275854
Entry Date (DED):	2001/07/25
Update Date (DUPD):	2007/02/05



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1

```
     RXPRO     Substance is Reaction Product              1


=> d rx l39 6


L39  ANSWER 6 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX
     Reaction ID (.ID):              8765119
     Reactant BRN (.RBRN):           8786746, 507983
     Reactant (.RCT):                8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
                                     hthalazin-5-one, isocyanatocyclohexane
     Product BRN (.PBRN):            8806911
     Product (.PRO):                 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                                     ,5-g>phthalazine-6-carboxylic acid
                                     cyclohexylamide
     No. of React. Details (.NVAR):  1

Reaction Details:
RX
     Reaction RID (.RID):            8765119.1
     Reaction Classification (.CL):  Preparation
     Reagent (.RGT):                 Et3N
     Solvent (.SOL):                 CH2Cl2
     Time (.TIM):                    36 hour(s)
     Temperature (.T):               20 Cel
     Reaction Type (.TYP):           Addition
     Reference(s):
     1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
        Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
        De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
        BABS-6281753
     2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
        Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
        De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
        BABS-6592638

Reaction:
RX
     Reaction ID (.ID):              8790320
     Reactant BRN (.RBRN):           8806911
     Reactant (.RCT):                8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                                     ,5-g>phthalazine-6-carboxylic acid
                                     cyclohexylamide
     Product BRN (.PBRN):            8805983
     Product (.PRO):                 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                                     ,5-g>phthalazine-6-carboxylic acid
                                     cyclohexylamide
     No. of React. Details (.NVAR):  1

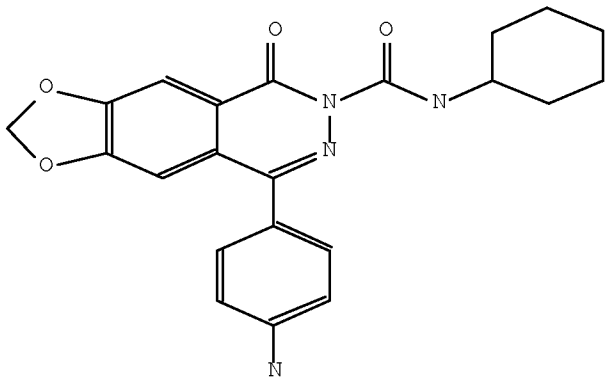
Reaction Details:
RX
     Reaction RID (.RID):            8790320.1
     Reaction Classification (.CL):  Preparation
     Yield (.YDT):                   231 mg (BRN=8805983)
     Reagent (.RGT):                 H2
     Catalyst (.CAT):                5 percent Pd/C
     Solvent (.SOL):                 methanol
```

Time (.TIM): 3 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Catalytic hydrogenation
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide l39 7

L39 ANSWER 7 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8805983
Chemical Name (CN): 4-(4-aminophenyl)-2-cyclohexylcarbamoyl-6,7-methylenedioxyphthalazin-1(2H)-one
Autonom Name (AUN): 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid cyclohexylamide
Molec. Formula (MF): C22 H22 N4 O4
Molecular Weight (MW): 406.44
Lawson Number (LN): 32399, 14011, 1762
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 7454782
Tautomer ID (TAUTID): 8283445
Entry Date (DED): 2001/07/25
Update Date (DUPD): 2007/02/05



Field Availability:

Code Name Occurrence

BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	5
PHARM	Pharmacological Data	4

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 7

L39 ANSWER 7 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	8790320
Reactant BRN (.RBRN):	8806911
Reactant (.RCT):	8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid cyclohexylamide
Product BRN (.PBRN):	8805983
Product (.PRO):	8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid cyclohexylamide
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	8790320.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	231 mg (BRN=8805983)
Reagent (.RGT):	H2
Catalyst (.CAT):	5 percent Pd/C
Solvent (.SOL):	methanol
Time (.TIM):	3 hour(s)
Temperature (.T):	20 Cel
Reaction Type (.TYP):	Catalytic hydrogenation

Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,

Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

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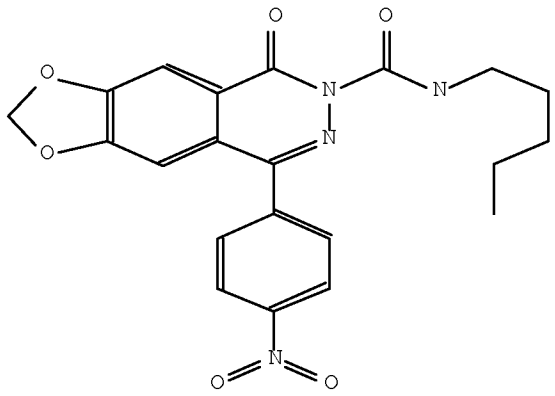
L39 ANSWER 8 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	8805084
Chemical Name (CN):	8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid pentylamide
Autonom Name (AUN):	8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid pentylamide
Molec. Formula (MF):	C21 H20 N4 O6
Molecular Weight (MW):	424.41
Lawson Number (LN):	32359, 2853, 1762
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7454058
Tautomer ID (TAUTID):	8274795
Entry Date (DED):	2001/07/25
Update Date (DUPD):	2007/02/05



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1

TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 8

L39 ANSWER 8 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	8748671
Reactant BRN (.RBRN):	8786746, 1746688
Reactant (.RCT):	8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one, pentyl isocyanate
Product BRN (.PBRN):	8805084
Product (.PRO):	8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid pentylamide
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	8748671.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	Et3N
Solvent (.SOL):	CH2Cl2
Time (.TIM):	36 hour(s)
Temperature (.T):	20 Cel
Reaction Type (.TYP):	Addition

Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:
RX

Reaction ID (.ID):	8789734
Reactant BRN (.RBRN):	8805084
Reactant (.RCT):	8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid pentylamide
Product BRN (.PBRN):	8802703
Product (.PRO):	8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid pentylamide

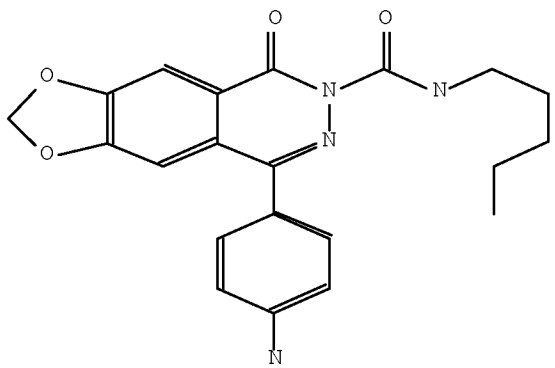
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 8789734.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 255 mg (BRN=8802703)
Reagent (.RGT): H2
Catalyst (.CAT): 5 percent Pd/C
Solvent (.SOL): methanol
Time (.TIM): 3 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Catalytic hydrogenation
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide l39 9

L39 ANSWER 9 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8802703
Chemical Name (CN): 4-(4-aminophenyl)-6,7-methylenedioxy-2-pentylcarbamoylphthalazin-1(2H)-one
Autonom Name (AUN): 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid pentylamide
Molec. Formula (MF): C21 H22 N4 O4
Molecular Weight (MW): 394.43
Lawson Number (LN): 32399, 2853, 1762
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 7452174
Tautomer ID (TAUTID): 8281628
Entry Date (DED): 2001/07/25
Update Date (DUPD): 2007/02/05



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
MP	Melting Point	1
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	5
PHARM	Pharmacological Data	4

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 9

L39 ANSWER 9 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	8789734
Reactant BRN (.RBRN):	8805084
Reactant (.RCT):	8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid pentylamide
Product BRN (.PBRN):	8802703
Product (.PRO):	8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid pentylamide
No. of React. Details (.NVAR):	1

Reaction Details:
RX

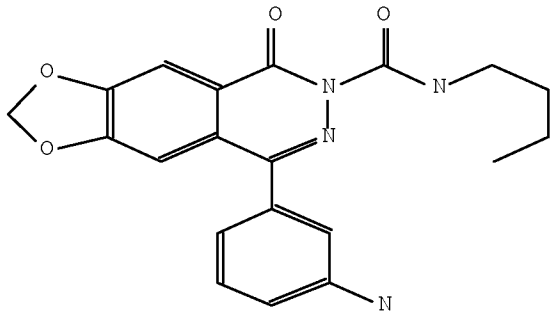
Reaction RID (.RID):	8789734.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	255 mg (BRN=8802703)
Reagent (.RGT):	H2
Catalyst (.CAT):	5 percent Pd/C
Solvent (.SOL):	methanol
Time (.TIM):	3 hour(s)
Temperature (.T):	20 Cel

Reaction Type (.TYP): Catalytic hydrogenation
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide l39 10

L39 ANSWER 10 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	8802426
Chemical Name (CN):	4-(3-aminophenyl)-2-butylcarbamoyl-6,7-methylenedioxyphthalazin-1(2H)-one
Autonom Name (AUN):	8-(3-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid butylamide
Molec. Formula (MF):	C20 H20 N4 O4
Molecular Weight (MW):	380.40
Lawson Number (LN):	32399, 2844, 1762
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7451936
Tautomer ID (TAUTID):	8288967
Entry Date (DED):	2001/07/25
Update Date (DUPD):	2007/02/05



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3

CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
MP	Melting Point	1
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	5
PHARM	Pharmacological Data	4

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 10

L39 ANSWER 10 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	8788563
Reactant BRN (.RBRN):	8801393
Reactant (.RCT):	8-(3-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid butylamide
Product BRN (.PBRN):	8802426
Product (.PRO):	8-(3-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid butylamide
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	8788563.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	250 mg (BRN=8802426)
Reagent (.RGT):	H2
Catalyst (.CAT):	5 percent Pd/C
Solvent (.SOL):	methanol
Time (.TIM):	3 hour(s)
Temperature (.T):	20 Cel
Reaction Type (.TYP):	Catalytic hydrogenation

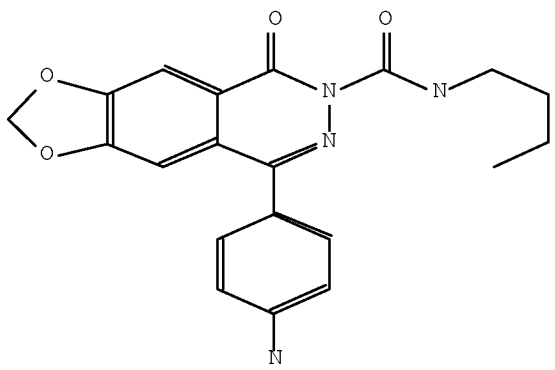
Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide l39 11

L39 ANSWER 11 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	8801464
Chemical Name (CN):	4-(4-aminophenyl)-2-butylcarbamoyl-6,7-methylenedioxyphthalazin-1(2H)-one
Autonom Name (AUN):	8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid butylamide
Molec. Formula (MF):	C20 H20 N4 O4
Molecular Weight (MW):	380.40
Lawson Number (LN):	32399, 2844, 1762
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7451143
Tautomer ID (TAUTID):	8280453
Entry Date (DED):	2001/07/25
Update Date (DUPD):	2007/02/05



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	5
PHARM	Pharmacological Data	26

This substance also occurs in Reaction Documents:

Code	Name	Occurrence

```
     ========================================================
     RX        Reaction Documents                          1
     RXPRO     Substance is Reaction Product               1


=> d rx l39 11


L39  ANSWER 11 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX
     Reaction ID (.ID):              8788551
     Reactant BRN (.RBRN):           8801355
     Reactant (.RCT):                8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                                     ,5-g>phthalazine-6-carboxylic acid
                                     butylamide
     Product BRN (.PBRN):            8801464
     Product (.PRO):                 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                                     ,5-g>phthalazine-6-carboxylic acid
                                     butylamide
     No. of React. Details (.NVAR):  1

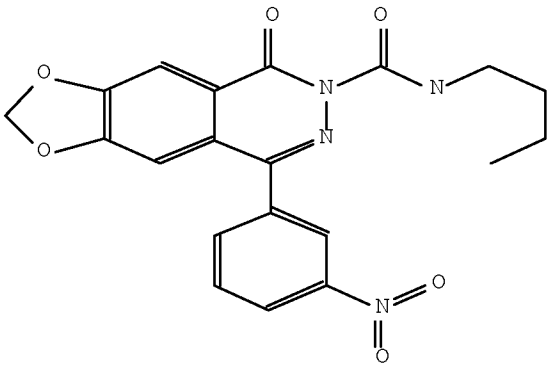
Reaction Details:
RX
     Reaction RID (.RID):            8788551.1
     Reaction Classification (.CL):  Preparation
     Yield (.YDT):                   261 mg (BRN=8801464)
     Reagent (.RGT):                 H2
     Catalyst (.CAT):                5 percent Pd/C
     Solvent (.SOL):                 methanol
     Time (.TIM):                    3 hour(s)
     Temperature (.T):               20 Cel
     Reaction Type (.TYP):           Catalytic hydrogenation
     Reference(s):
     1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
        Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
        De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
        BABS-6281753
     2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
        Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
        De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
        BABS-6592638


=> d ide l39 12


L39  ANSWER 12 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

     Beilstein Records (BRN):        8801393
     Chemical Name (CN):             8-(3-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                                     ,5-g>phthalazine-6-carboxylic acid
                                     butylamide
     Autonom Name (AUN):             8-(3-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                                     ,5-g>phthalazine-6-carboxylic acid
                                     butylamide
     Molec. Formula (MF):            C20 H18 N4 O6
     Molecular Weight (MW):          410.39
     Lawson Number (LN):             32359, 2844, 1762
```

Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 7451080
Tautomer ID (TAUTID): 8271672
Entry Date (DED): 2001/07/25
Update Date (DUPD): 2007/02/05



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 12

L39 ANSWER 12 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX
Reaction ID (.ID): 8774333
Reactant BRN (.RBRN): 8787337, 773917

Reactant (.RCT): 8-(3-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one, 1-isocyanato-butane
Product BRN (.PBRN): 8801393
Product (.PRO): 8-(3-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid butylamide
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 8774333.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): Et3N
Solvent (.SOL): CH2Cl2
Time (.TIM): 36 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Addition
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:
RX
Reaction ID (.ID): 8788563
Reactant BRN (.RBRN): 8801393
Reactant (.RCT): 8-(3-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid butylamide
Product BRN (.PBRN): 8802426
Product (.PRO): 8-(3-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid butylamide
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 8788563.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 250 mg (BRN=8802426)
Reagent (.RGT): H2
Catalyst (.CAT): 5 percent Pd/C
Solvent (.SOL): methanol
Time (.TIM): 3 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Catalytic hydrogenation
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

```
=> d ide l39 13

L39  ANSWER 13 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

     Beilstein Records (BRN):        8801355
     Chemical Name (CN):             8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                                     ,5-g>phthalazine-6-carboxylic acid
                                     butylamide
     Autonom Name (AUN):             8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                                     ,5-g>phthalazine-6-carboxylic acid
                                     butylamide
     Molec. Formula (MF):            C20 H18 N4 O6
     Molecular Weight (MW):          410.39
     Lawson Number (LN):             32359, 2844, 1762
     Compound Type (CTYPE):          heterocyclic
     Constitution ID (CONSID):       7451041
     Tautomer ID (TAUTID):           8271733
     Entry Date (DED):               2001/07/25
     Update Date (DUPD):             2007/02/05
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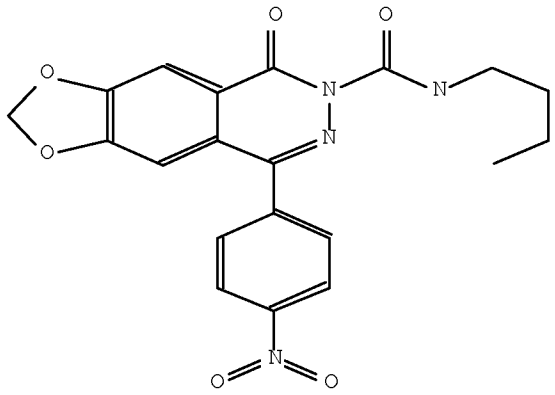


Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 13

L39 ANSWER 13 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	8774332
Reactant BRN (.RBRN):	8786746, 773917
Reactant (.RCT):	8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one, 1-isocyanato-butane
Product BRN (.PBRN):	8801355
Product (.PRO):	8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid butylamide
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	8774332.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	Et3N
Solvent (.SOL):	CH2Cl2
Time (.TIM):	36 hour(s)
Temperature (.T):	20 Cel
Reaction Type (.TYP):	Addition

Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:
RX

Reaction ID (.ID):	8788551
Reactant BRN (.RBRN):	8801355
Reactant (.RCT):	8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid butylamide
Product BRN (.PBRN):	8801464
Product (.PRO):	8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid butylamide
No. of React. Details (.NVAR):	1

Reaction Details:

RX

Reaction RID (.RID):	8788551.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	261 mg (BRN=8801464)
Reagent (.RGT):	H2
Catalyst (.CAT):	5 percent Pd/C
Solvent (.SOL):	methanol
Time (.TIM):	3 hour(s)
Temperature (.T):	20 Cel
Reaction Type (.TYP):	Catalytic hydrogenation

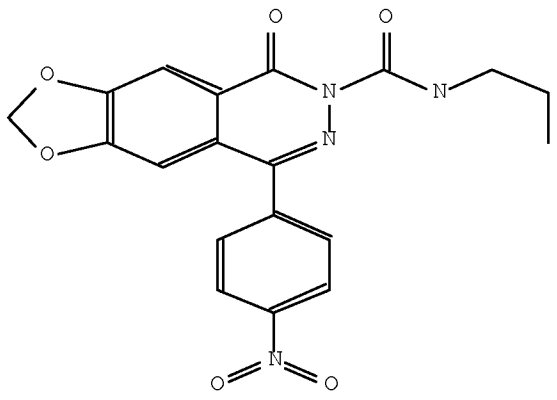
Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide l39 14

L39 ANSWER 14 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	8800760
Chemical Name (CN):	8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid propylamide
Autonom Name (AUN):	8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid propylamide
Molec. Formula (MF):	C19 H16 N4 O6
Molecular Weight (MW):	396.36
Lawson Number (LN):	32359, 2835, 1762
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7450482
Tautomer ID (TAUTID):	8270366
Entry Date (DED):	2001/07/25
Update Date (DUPD):	2007/02/05



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 14

L39 ANSWER 14 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	8741512
Reactant BRN (.RBRN):	8786746, 1098489
Reactant (.RCT):	8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one, 1-isocyanato-propane
Product BRN (.PBRN):	8800760
Product (.PRO):	8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid propylamide
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	8741512.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	Et3N
Solvent (.SOL):	CH2Cl2
Time (.TIM):	36 hour(s)
Temperature (.T):	20 Cel
Reaction Type (.TYP):	Addition

Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753

2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:
RX

Reaction ID (.ID):	8788377
Reactant BRN (.RBRN):	8800760
Reactant (.RCT):	8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid propylamide
Product BRN (.PBRN):	8799445
Product (.PRO):	8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid propylamide
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	8788377.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	268 mg (BRN=8799445)
Reagent (.RGT):	H2
Catalyst (.CAT):	5 percent Pd/C
Solvent (.SOL):	methanol
Time (.TIM):	3 hour(s)
Temperature (.T):	20 Cel
Reaction Type (.TYP):	Catalytic hydrogenation

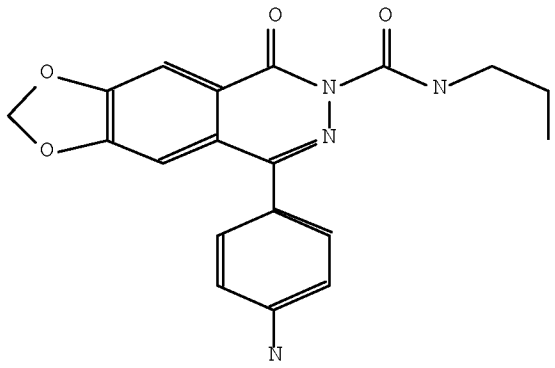
Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide l39 15

L39 ANSWER 15 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	8799445
Chemical Name (CN):	4-(4-aminophenyl)-6,7-methylenedioxy-2-propylcarbamoylphthalazin-1(2H)-one
Autonom Name (AUN):	8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid propylamide
Molec. Formula (MF):	C19 H18 N4 O4
Molecular Weight (MW):	366.38
Lawson Number (LN):	32399, 2835, 1762
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7449368
Tautomer ID (TAUTID):	8279684
Entry Date (DED):	2001/07/25
Update Date (DUPD):	2007/02/05



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	5
PHARM	Pharmacological Data	4

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 15

L39 ANSWER 15 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	8788377
Reactant BRN (.RBRN):	8800760
Reactant (.RCT):	8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid propylamide
Product BRN (.PBRN):	8799445

```
     Product (.PRO):                 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                                     ,5-g>phthalazine-6-carboxylic acid
                                     propylamide
     No. of React. Details (.NVAR):  1

Reaction Details:
RX
     Reaction RID (.RID):            8788377.1
     Reaction Classification (.CL):  Preparation
     Yield (.YDT):                   268 mg (BRN=8799445)
     Reagent (.RGT):                 H2
     Catalyst (.CAT):                5 percent Pd/C
     Solvent (.SOL):                 methanol
     Time (.TIM):                    3 hour(s)
     Temperature (.T):               20 Cel
     Reaction Type (.TYP):           Catalytic hydrogenation
     Reference(s):
     1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
        Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
        De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
        BABS-6281753
     2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
        Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
        De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
        BABS-6592638


=> d ide l39 16


L39  ANSWER 16 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

     Beilstein Records (BRN):        8798692
     Chemical Name (CN):             8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                                     ,5-g>phthalazine-6-carboxylic acid
                                     ethylamide
     Autonom Name (AUN):             8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                                     ,5-g>phthalazine-6-carboxylic acid
                                     ethylamide
     Molec. Formula (MF):            C18 H14 N4 O6
     Molecular Weight (MW):          382.33
     Lawson Number (LN):             32359, 2826, 1762
     Compound Type (CTYPE):          heterocyclic
     Constitution ID (CONSID):       7448692
     Tautomer ID (TAUTID):           8270132
     Entry Date (DED):               2001/07/25
     Update Date (DUPD):             2007/02/05
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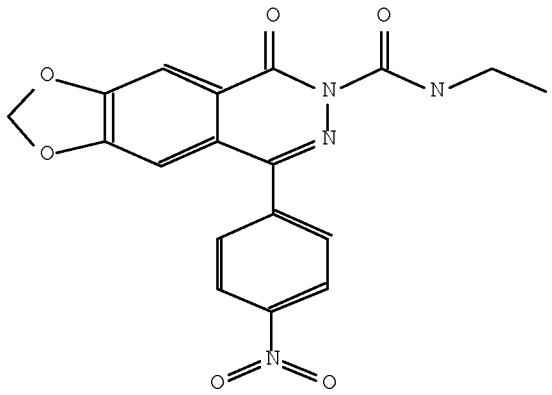

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 16

L39 ANSWER 16 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	8774240
Reactant BRN (.RBRN):	8786746, 773743
Reactant (.RCT):	8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one, isocyanatoethane
Product BRN (.PBRN):	8798692
Product (.PRO):	8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid ethylamide
No. of React. Details (.NVAR):	1

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Reaction Details:
RX
     Reaction RID (.RID):            8774240.1
     Reaction Classification (.CL):  Preparation
     Reagent (.RGT):                 Et3N
     Solvent (.SOL):                 CH2Cl2
     Time (.TIM):                    36 hour(s)
     Temperature (.T):               20 Cel
     Reaction Type (.TYP):           Addition
     Reference(s):
     1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
        Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
        De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
        BABS-6281753
     2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
        Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
        De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
        BABS-6592638

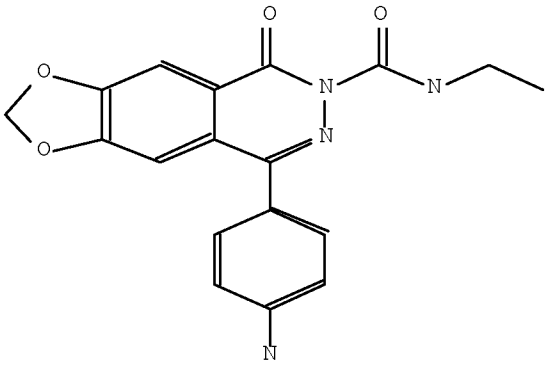
Reaction:
RX
     Reaction ID (.ID):              8787810
     Reactant BRN (.RBRN):           8798692
     Reactant (.RCT):                8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                                     ,5-g>phthalazine-6-carboxylic acid
                                     ethylamide
     Product BRN (.PBRN):            8797201
     Product (.PRO):                 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                                     ,5-g>phthalazine-6-carboxylic acid
                                     ethylamide
     No. of React. Details (.NVAR):  1

Reaction Details:
RX
     Reaction RID (.RID):            8787810.1
     Reaction Classification (.CL):  Preparation
     Yield (.YDT):                   272 mg (BRN=8797201)
     Reagent (.RGT):                 H2
     Catalyst (.CAT):                5 percent Pd/C
     Solvent (.SOL):                 methanol
     Time (.TIM):                    3 hour(s)
     Temperature (.T):               20 Cel
     Reaction Type (.TYP):           Catalytic hydrogenation
     Reference(s):
     1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
        Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
        De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
        BABS-6281753
     2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
        Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
        De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
        BABS-6592638


=> d ide l39 17


L39  ANSWER 17 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN
```

Beilstein Records (BRN):	8797201
Chemical Name (CN):	4-(4-aminophenyl)-2-ethylcarbamoyl-6,7-methylenedioxyphthalazin-1(2H)-one
Autonom Name (AUN):	8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid ethylamide
Molec. Formula (MF):	C18 H16 N4 O4
Molecular Weight (MW):	352.35
Lawson Number (LN):	32399, 2826, 1762
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7447398
Tautomer ID (TAUTID):	8277448
Entry Date (DED):	2001/07/25
Update Date (DUPD):	2007/02/05



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	5
PHARM	Pharmacological Data	4

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1

RXPRO Substance is Reaction Product 1

=> d rx l39 17

L39 ANSWER 17 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX
Reaction ID (.ID): 8787810
Reactant BRN (.RBRN): 8798692
Reactant (.RCT): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid ethylamide
Product BRN (.PBRN): 8797201
Product (.PRO): 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid ethylamide
No. of React. Details (.NVAR): 1

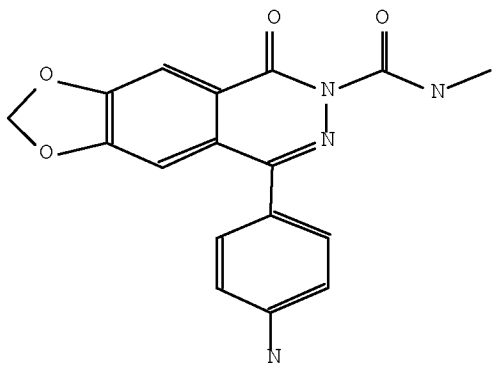
Reaction Details:
RX
Reaction RID (.RID): 8787810.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 272 mg (BRN=8797201)
Reagent (.RGT): H2
Catalyst (.CAT): 5 percent Pd/C
Solvent (.SOL): methanol
Time (.TIM): 3 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Catalytic hydrogenation
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide l39 18

L39 ANSWER 18 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8796253
Chemical Name (CN): 4-(4-aminophenyl)-2-methylcarbamoyl-6,7-methylenedioxyphthalazin-1(2H)-one
Autonom Name (AUN): 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid methylamide
Molec. Formula (MF): C17 H14 N4 O4
Molecular Weight (MW): 338.32
Lawson Number (LN): 32399, 2817, 1762
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 7446672
Tautomer ID (TAUTID): 8276307

Entry Date (DED): 2001/07/25
Update Date (DUPD): 2007/02/05



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	5
PHARM	Pharmacological Data	4

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 18

L39 ANSWER 18 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX
Reaction ID (.ID): 8787000
Reactant BRN (.RBRN): 8795870
Reactant (.RCT): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4

,5-g>phthalazine-6-carboxylic acid methylamide

Product BRN (.PBRN): 8796253

Product (.PRO): 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid methylamide

No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 8787000.1

Reaction Classification (.CL): Preparation

Yield (.YDT): 239 mg (BRN=8796253)

Reagent (.RGT): H2

Catalyst (.CAT): 5 percent Pd/C

Solvent (.SOL): methanol

Time (.TIM): 3 hour(s)

Temperature (.T): 20 Cel

Reaction Type (.TYP): Catalytic hydrogenation

Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide l39 19

L39 ANSWER 19 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8795870

Chemical Name (CN): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid methylamide

Autonom Name (AUN): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid methylamide

Molec. Formula (MF): C17 H12 N4 O6

Molecular Weight (MW): 368.31

Lawson Number (LN): 32359, 2817, 1762

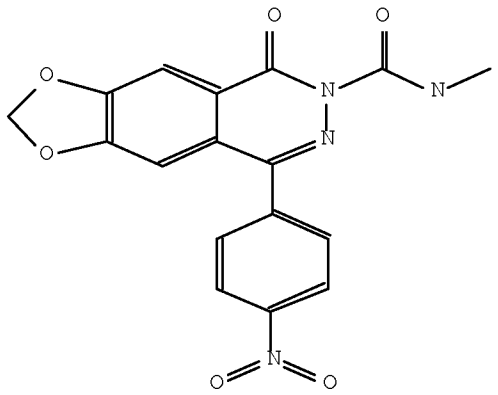
Compound Type (CTYPE): heterocyclic

Constitution ID (CONSID): 7446283

Tautomer ID (TAUTID): 8266541

Entry Date (DED): 2001/07/25

Update Date (DUPD): 2007/02/05



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 19

L39 ANSWER 19 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	8767356
Reactant BRN (.RBRN):	8786746, 605318
Reactant (.RCT):	8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one, isocyanatomethane
Product BRN (.PBRN):	8795870
Product (.PRO):	8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid methylamide
No. of React. Details (.NVAR):	1

Reaction Details:
RX
Reaction RID (.RID): 8767356.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): Et3N
Solvent (.SOL): CH2Cl2
Time (.TIM): 36 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Addition
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

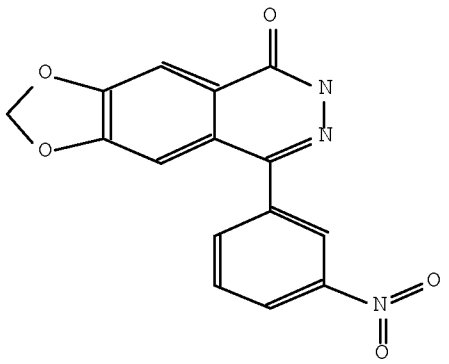
Reaction:
RX
Reaction ID (.ID): 8787000
Reactant BRN (.RBRN): 8795870
Reactant (.RCT): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid methylamide
Product BRN (.PBRN): 8796253
Product (.PRO): 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid methylamide
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 8787000.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 239 mg (BRN=8796253)
Reagent (.RGT): H2
Catalyst (.CAT): 5 percent Pd/C
Solvent (.SOL): methanol
Time (.TIM): 3 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Catalytic hydrogenation
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide l39 20

L39 ANSWER 20 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	8787337
Chemical Name (CN):	6,7-methylenedioxy-4-(3-nitrophenyl)-phthalazin-1(2H)-one
Autonom Name (AUN):	8-(3-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
Molec. Formula (MF):	C15 H9 N3 O5
Molecular Weight (MW):	311.25
Lawson Number (LN):	32359
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7439055
Tautomer ID (TAUTID):	8280617
Entry Date (DED):	2001/07/25
Update Date (DUPD):	2007/02/05



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
NMR	Nuclear Magnetic Resonance	5

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3
RXREA	Substance is Reaction Reactant	2
RXPRO	Substance is Reaction Product	1

```
=> d rx l39 20


L39  ANSWER 20 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX
     Reaction ID (.ID):              8782108
     Reactant BRN (.RBRN):           8778660
     Reactant (.RCT):                (6-methyl-benzo<1,3>dioxol-5-yl)-(3-nitro-
                                     phenyl)-methanone
     Product BRN (.PBRN):            8787337
     Product (.PRO):                 8-(3-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
                                     hthalazin-5-one
     No. of React. Details (.NVAR):  2

Reaction Details:
RX
     Reaction RID (.RID):            8782108.1
     Reaction Classification (.CL):  Multistage
     Yield (.YDT):                   52 percent (BRN=8787337)
     Nr. of Stages (.SNR):           2
     Stage 1
     Reagent (.RGT):                 bromine
     Solvent (.SOL):                 CCl4
     Time (.TIM):                    8 hour(s)
     Other Conditions (.COND):       Heating, UV-irradiation
     Reaction Type (.TYP):           Bromination
     Stage 2
     Reagent (.RGT):                 NH2NH2*H2O
     Solvent (.SOL):                 ethanol
     Temperature (.T):               16 Cel
     Other Conditions (.COND):       Heating
     Reaction Type (.TYP):           Oxidation, cyclocondensation
     Reference(s):
     1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
        Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
        De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
        BABS-6592638
RX
     Reaction RID (.RID):            8782108.2
     Reaction Classification (.CL):  Multistage
     Yield (.YDT):                   52 percent (BRN=8787337)
     Nr. of Stages (.SNR):           2
     Stage 1
     Reagent (.RGT):                 bromine
     Solvent (.SOL):                 CCl4
     Time (.TIM):                    8 hour(s)
     Other Conditions (.COND):       Heating, UV-irradiation
     Reaction Type (.TYP):           Bromination, Oxidation
     Stage 2
     Reagent (.RGT):                 NH2NH2*H2O
     Solvent (.SOL):                 ethanol
     Temperature (.T):               16 Cel
     Other Conditions (.COND):       Heating
     Reaction Type (.TYP):           cyclocondensation
     Reference(s):
     1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
```

Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753

Reaction:
RX
Reaction ID (.ID): 8784730
Reactant BRN (.RBRN): 8787337
Reactant (.RCT): 8-(3-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
Product BRN (.PBRN): 8786723
Product (.PRO): 8-(3-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 8784730.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 87 percent (BRN=8786723)
Reagent (.RGT): H2
Catalyst (.CAT): 5 percent Pd/C
Solvent (.SOL): methanol
Time (.TIM): 3 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Catalytic hydrogenation
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:
RX
Reaction ID (.ID): 8774333
Reactant BRN (.RBRN): 8787337, 773917
Reactant (.RCT): 8-(3-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one, 1-isocyanato-butane
Product BRN (.PBRN): 8801393
Product (.PRO): 8-(3-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid butylamide
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 8774333.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): Et3N
Solvent (.SOL): CH2Cl2
Time (.TIM): 36 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Addition
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo

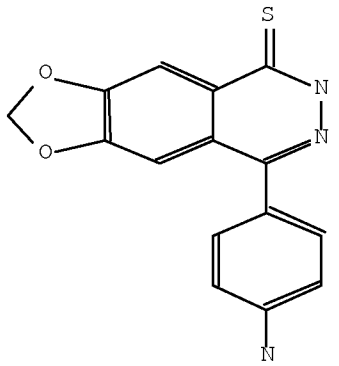
De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753

2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide l39 21

L39 ANSWER 21 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	8786898
Chemical Name (CN):	4-(4-aminophenyl)-6,7-methylenedioxyphthalazine-1(2H)-thione
Autonom Name (AUN):	8-(4-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazine-5-thione
Molec. Formula (MF):	C15 H11 N3 O2 S
Molecular Weight (MW):	297.33
Lawson Number (LN):	32394
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7438673
Tautomer ID (TAUTID):	8279184
Entry Date (DED):	2001/07/25
Update Date (DUPD):	2007/02/05



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1

CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
NMR	Nuclear Magnetic Resonance	5
PHARM	Pharmacological Data	4

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 21

L39 ANSWER 21 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	8784559
Reactant BRN (.RBRN):	8786694
Reactant (.RCT):	8-(4-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
Product BRN (.PBRN):	8786898
Product (.PRO):	8-(4-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazine-5-thione
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	8784559.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	82 percent (BRN=8786898)
Reagent (.RGT):	Lawesson's reagent
Solvent (.SOL):	toluene
Time (.TIM):	2 hour(s)
Other Conditions (.COND):	Heating
Reaction Type (.TYP):	Substitution

Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

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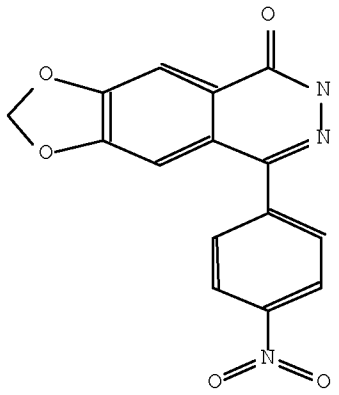
L39 ANSWER 22 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	8786746
Chemical Name (CN):	6,7-methylenedioxy-4-(4-nitrophenyl)-phthalazin-1(2H)-one

Autonom Name (AUN):	8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
Molec. Formula (MF):	C15 H9 N3 O5
Molecular Weight (MW):	311.25
Lawson Number (LN):	32359
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7438558
Tautomer ID (TAUTID):	8281644
Entry Date (DED):	2001/07/25
Update Date (DUPD):	2007/02/05



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	5
PHARM	Pharmacological Data	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	10
RXREA	Substance is Reaction Reactant	8
RXPRO	Substance is Reaction Product	2

```
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L39  ANSWER 22 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX
     Reaction ID (.ID):              9460950
     Reactant BRN (.RBRN):           331047
     Reactant (.RCT):                6-(4-nitro-benzoyl)-benzo<1,3>dioxole-5-ca
                                     rboxylic acid
     Product BRN (.PBRN):            8786746
     Product (.PRO):                 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
                                     hthalazin-5-one
     No. of React. Details (.NVAR):  1

Reaction Details:
RX
     Reaction RID (.RID):            9460950.1
     Reaction Classification (.CL):  Preparation
     Reagent (.RGT):                 aq. H2NNH2
     Solvent (.SOL):                 ethanol
     Other Conditions (.COND):       Heating
     Reference(s):
     1. Solyom, Sandor; Hamori, Tamas; Borosy, Andras P.; Tarnawa, Istvan;
        Bersenyi, Pal; Pallagi, Istvan, Med.Chem.Res., CODEN: MCREEB, 11(1),
        <2002>, 39 - 49; BABS-6420582

Reaction:
RX
     Reaction ID (.ID):              8782107
     Reactant BRN (.RBRN):           8778659
     Reactant (.RCT):                (6-methyl-benzo<1,3>dioxol-5-yl)-(4-nitro-
                                     phenyl)-methanone
     Product BRN (.PBRN):            8786746
     Product (.PRO):                 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
                                     hthalazin-5-one
     No. of React. Details (.NVAR):  2

Reaction Details:
RX
     Reaction RID (.RID):            8782107.1
     Reaction Classification (.CL):  Multistage
     Yield (.YDT):                   55 percent (BRN=8786746)
     Nr. of Stages (.SNR):           2
     Stage 1
     Reagent (.RGT):                 bromine
     Solvent (.SOL):                 CCl4
     Time (.TIM):                    8 hour(s)
     Other Conditions (.COND):       Heating, UV-irradiation
     Reaction Type (.TYP):           Bromination
     Stage 2
     Reagent (.RGT):                 NH2NH2*H2O
     Solvent (.SOL):                 ethanol
     Temperature (.T):               16 Cel
     Other Conditions (.COND):       Heating
     Reaction Type (.TYP):           Oxidation, cyclocondensation
     Reference(s):
```

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

RX

Reaction RID (.RID):	8782107.2
Reaction Classification (.CL):	Multistage
Yield (.YDT):	55 percent (BRN=8786746)
Nr. of Stages (.SNR):	2
Stage 1	
Reagent (.RGT):	bromine
Solvent (.SOL):	CCl4
Time (.TIM):	8 hour(s)
Other Conditions (.COND):	Heating, UV-irradiation
Reaction Type (.TYP):	Bromination, Oxidation
Stage 2	
Reagent (.RGT):	NH2NH2*H2O
Solvent (.SOL):	ethanol
Temperature (.T):	16 Cel
Other Conditions (.COND):	Heating
Reaction Type (.TYP):	cyclocondensation
Reference(s):	

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753

Reaction:

RX

Reaction ID (.ID):	9481786
Reactant BRN (.RBRN):	8786746
Reactant (.RCT):	8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
Product BRN (.PBRN):	9575008
Product (.PRO):	5-chloro-8-(4-nitro-phenyl)-<1,3>dioxolo<4,5-g>phthalazine
No. of React. Details (.NVAR):	1

Reaction Details:

RX

Reaction RID (.RID):	9481786.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	POCl3
Other Conditions (.COND):	Heating
Reference(s):	

1. Solyom, Sandor; Hamori, Tamas; Borosy, Andras P.; Tarnawa, Istvan; Bersenyi, Pal; Pallagi, Istvan, Med.Chem.Res., CODEN: MCREEB, 11(1), <2002>, 39 - 49; BABS-6420582

Reaction:

RX

Reaction ID (.ID):	8784574
Reactant BRN (.RBRN):	8786746
Reactant (.RCT):	8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
Product BRN (.PBRN):	8786694
Product (.PRO):	8-(4-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
No. of React. Details (.NVAR):	1

Reaction Details:
RX
Reaction RID (.RID): 8784574.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 89 percent (BRN=8786694)
Reagent (.RGT): H2
Catalyst (.CAT): 5 percent Pd/C
Solvent (.SOL): methanol
Time (.TIM): 3 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Catalytic hydrogenation
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:
RX
Reaction ID (.ID): 8774332
Reactant BRN (.RBRN): 8786746, 773917
Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one, 1-isocyanato-butane
Product BRN (.PBRN): 8801355
Product (.PRO): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid butylamide
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 8774332.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): Et3N
Solvent (.SOL): CH2Cl2
Time (.TIM): 36 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Addition
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:
RX
Reaction ID (.ID): 8774240
Reactant BRN (.RBRN): 8786746, 773743
Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one, isocyanatoethane
Product BRN (.PBRN): 8798692
Product (.PRO): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4

,5-g>phthalazine-6-carboxylic acid ethylamide
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 8774240.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): Et3N
Solvent (.SOL): CH2Cl2
Time (.TIM): 36 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Addition
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:
RX
Reaction ID (.ID): 8767356
Reactant BRN (.RBRN): 8786746, 605318
Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one, isocyanatomethane
Product BRN (.PBRN): 8795870
Product (.PRO): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid methylamide
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 8767356.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): Et3N
Solvent (.SOL): CH2Cl2
Time (.TIM): 36 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Addition
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:
RX
Reaction ID (.ID): 8765119
Reactant BRN (.RBRN): 8786746, 507983
Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one, isocyanatocyclohexane

Product BRN (.PBRN): 8806911
Product (.PRO): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid cyclohexylamide
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 8765119.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): Et3N
Solvent (.SOL): CH2Cl2
Time (.TIM): 36 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Addition
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:
RX
Reaction ID (.ID): 8748671
Reactant BRN (.RBRN): 8786746, 1746688
Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one, pentyl isocyanate
Product BRN (.PBRN): 8805084
Product (.PRO): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid pentylamide
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 8748671.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): Et3N
Solvent (.SOL): CH2Cl2
Time (.TIM): 36 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Addition
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:
RX
Reaction ID (.ID): 8741512
Reactant BRN (.RBRN): 8786746, 1098489

```
     Reactant (.RCT):                8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
                                     hthalazin-5-one, 1-isocyanato-propane
     Product BRN (.PBRN):            8800760
     Product (.PRO):                 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                                     ,5-g>phthalazine-6-carboxylic acid
                                     propylamide
     No. of React. Details (.NVAR):  1

Reaction Details:
RX
     Reaction RID (.RID):            8741512.1
     Reaction Classification (.CL):  Preparation
     Reagent (.RGT):                 Et3N
     Solvent (.SOL):                 CH2Cl2
     Time (.TIM):                    36 hour(s)
     Temperature (.T):               20 Cel
     Reaction Type (.TYP):           Addition
     Reference(s):
     1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
        Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
        De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
        BABS-6281753
     2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
        Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
        De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
        BABS-6592638


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     Beilstein Records (BRN):        8786723
     Chemical Name (CN):             4-(3-aminophenyl)-6,7-methylenedioxyphthal
                                     azin-1(2H)-one
     Autonom Name (AUN):             8-(3-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>p
                                     hthalazin-5-one
     Molec. Formula (MF):            C15 H11 N3 O3
     Molecular Weight (MW):          281.27
     Lawson Number (LN):             32399
     Compound Type (CTYPE):          heterocyclic
     Constitution ID (CONSID):       7438541
     Tautomer ID (TAUTID):           8278845
     Entry Date (DED):               2001/07/25
     Update Date (DUPD):             2007/02/05
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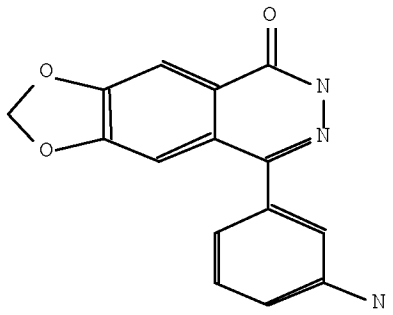

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	5
PHARM	Pharmacological Data	4

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

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L39 ANSWER 23 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	8784730
Reactant BRN (.RBRN):	8787337
Reactant (.RCT):	8-(3-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
Product BRN (.PBRN):	8786723
Product (.PRO):	8-(3-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
No. of React. Details (.NVAR):	1

Reaction Details:

RX

Reaction RID (.RID):	8784730.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	87 percent (BRN=8786723)
Reagent (.RGT):	H2
Catalyst (.CAT):	5 percent Pd/C
Solvent (.SOL):	methanol
Time (.TIM):	3 hour(s)
Temperature (.T):	20 Cel
Reaction Type (.TYP):	Catalytic hydrogenation

Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

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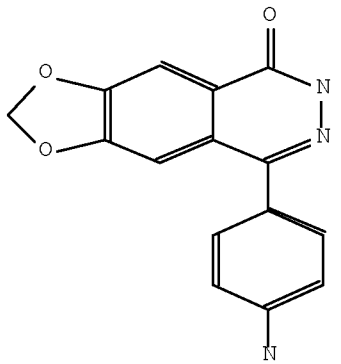
L39 ANSWER 24 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	8786694
Chemical Name (CN):	4-(4-aminophenyl)-6,7-methylenedioxyphthalazin-1(2H)-one
Autonom Name (AUN):	8-(4-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
Molec. Formula (MF):	C15 H11 N3 O3
Molecular Weight (MW):	281.27
Lawson Number (LN):	32399
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7438516
Tautomer ID (TAUTID):	8278888
Entry Date (DED):	2001/07/25
Update Date (DUPD):	2007/02/05



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
NMR	Nuclear Magnetic Resonance	5
PHARM	Pharmacological Data	28

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

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L39 ANSWER 24 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	8784574
Reactant BRN (.RBRN):	8786746
Reactant (.RCT):	8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
Product BRN (.PBRN):	8786694
Product (.PRO):	8-(4-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	8784574.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	89 percent (BRN=8786694)
Reagent (.RGT):	H2
Catalyst (.CAT):	5 percent Pd/C
Solvent (.SOL):	methanol
Time (.TIM):	3 hour(s)
Temperature (.T):	20 Cel
Reaction Type (.TYP):	Catalytic hydrogenation

Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;

BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:
RX
Reaction ID (.ID): 8784559
Reactant BRN (.RBRN): 8786694
Reactant (.RCT): 8-(4-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
Product BRN (.PBRN): 8786898
Product (.PRO): 8-(4-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazine-5-thione
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 8784559.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 82 percent (BRN=8786898)
Reagent (.RGT): Lawesson's reagent
Solvent (.SOL): toluene
Time (.TIM): 2 hour(s)
Other Conditions (.COND): Heating
Reaction Type (.TYP): Substitution
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

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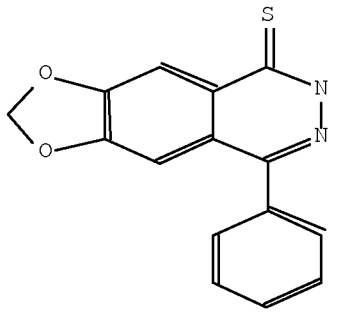
L39 ANSWER 25 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8780260
Chemical Name (CN): 6,7-methylenedioxy-4-phenylphthalazine-1(2H)-thione
Autonom Name (AUN): 8-phenyl-6H-<1,3>dioxolo<4,5-g>phthalazine-5-thione
Molec. Formula (MF): C15 H10 N2 O2 S
Molecular Weight (MW): 282.32
Lawson Number (LN): 32353
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 7432908
Tautomer ID (TAUTID): 8277944
Entry Date (DED): 2001/07/25
Update Date (DUPD): 2007/02/05



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	4
PHARM	Pharmacological Data	4

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 25

L39 ANSWER 25 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	8782500
Reactant BRN (.RBRN):	8780129
Reactant (.RCT):	8-phenyl-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
Product BRN (.PBRN):	8780260
Product (.PRO):	8-phenyl-6H-<1,3>dioxolo<4,5-g>phthalazine-5-thione
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	8782500.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	85 percent (BRN=8780260)
Reagent (.RGT):	Lawesson's reagent
Solvent (.SOL):	toluene
Time (.TIM):	2 hour(s)
Other Conditions (.COND):	Heating
Reaction Type (.TYP):	Substitution

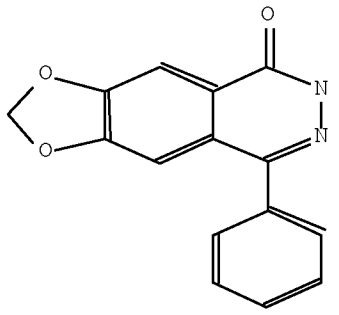
Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide l39 26

L39 ANSWER 26 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	8780129
Chemical Name (CN):	6,7-methylenedioxy-4-phenylphthalazin-1(2H)-one
Autonom Name (AUN):	8-phenyl-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
Molec. Formula (MF):	C15 H10 N2 O3
Molecular Weight (MW):	266.26
Lawson Number (LN):	32358
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7432813
Tautomer ID (TAUTID):	8277953
Entry Date (DED):	2001/07/25
Update Date (DUPD):	2007/02/05



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	4
PHARM	Pharmacological Data	4

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 26

L39 ANSWER 26 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	8766058
Reactant BRN (.RBRN):	5544914
Reactant (.RCT):	6-methylbenzo-1,3-dioxol-5-yl phenyl ketone
Product BRN (.PBRN):	8780129
Product (.PRO):	8-phenyl-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
No. of React. Details (.NVAR):	2

Reaction Details:
RX

Reaction RID (.RID):	8766058.1
Reaction Classification (.CL):	Multistage
Yield (.YDT):	59 percent (BRN=8780129)
Nr. of Stages (.SNR):	2
Stage 1	
Reagent (.RGT):	bromine
Solvent (.SOL):	CCl4
Time (.TIM):	8 hour(s)
Other Conditions (.COND):	Heating, UV-irradiation
Reaction Type (.TYP):	Bromination
Stage 2	
Reagent (.RGT):	NH2NH2*H2O
Solvent (.SOL):	ethanol
Temperature (.T):	16 Cel

```
     Other Conditions (.COND):       Heating
     Reaction Type (.TYP):           Oxidation, cyclocondensation
     Reference(s):
     1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
        Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
        De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
        BABS-6592638
RX
     Reaction RID (.RID):            8766058.2
     Reaction Classification (.CL):  Multistage
     Yield (.YDT):                   59 percent (BRN=8780129)
     Nr. of Stages (.SNR):           2
     Stage 1
     Reagent (.RGT):                 bromine
     Solvent (.SOL):                 CCl4
     Time (.TIM):                    8 hour(s)
     Other Conditions (.COND):       Heating, UV-irradiation
     Reaction Type (.TYP):           Bromination, Oxidation
     Stage 2
     Reagent (.RGT):                 NH2NH2*H2O
     Solvent (.SOL):                 ethanol
     Temperature (.T):               16 Cel
     Other Conditions (.COND):       Heating
     Reaction Type (.TYP):           cyclocondensation
     Reference(s):
     1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
        Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
        De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
        BABS-6281753

Reaction:
RX
     Reaction ID (.ID):              8782500
     Reactant BRN (.RBRN):           8780129
     Reactant (.RCT):                8-phenyl-6H-<1,3>dioxolo<4,5-g>phthalazin-
                                     5-one
     Product BRN (.PBRN):            8780260
     Product (.PRO):                 8-phenyl-6H-<1,3>dioxolo<4,5-g>phthalazine
                                     -5-thione
     No. of React. Details (.NVAR):  1

Reaction Details:
RX
     Reaction RID (.RID):            8782500.1
     Reaction Classification (.CL):  Preparation
     Yield (.YDT):                   85 percent (BRN=8780260)
     Reagent (.RGT):                 Lawesson's reagent
     Solvent (.SOL):                 toluene
     Time (.TIM):                    2 hour(s)
     Other Conditions (.COND):       Heating
     Reaction Type (.TYP):           Substitution
     Reference(s):
     1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
        Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
        De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
        BABS-6281753
     2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
        Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
        De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
        BABS-6592638
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=> d ide l39 27
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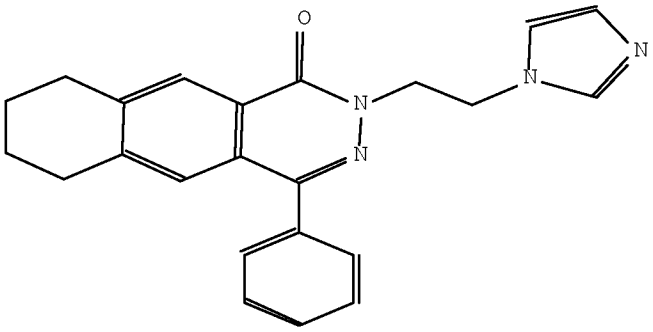
L39 ANSWER 27 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	8444536
Chemical Name (CN):	6,7,8,9-tetrahydro-2-<2-(1-imidazolyl)ethyl>-4-phenyl-benzo<g>phthalazin-1(2H)-one
Autonom Name (AUN):	2-(2-imidazol-1-yl-ethyl)-4-phenyl-6,7,8,9-tetrahydro-2H-benzo<g>phthalazin-1-one
Molec. Formula (MF):	C23 H22 N4 O
Molecular Weight (MW):	370.45
Lawson Number (LN):	28745, 28020, 3706
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7164599
Tautomer ID (TAUTID):	7965180
Entry Date (DED):	2000/05/16
Update Date (DUPD):	2000/05/16



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	2

Code	Name	Occurrence
PHARM	Pharmacological Data	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 27

L39 ANSWER 27 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	8533023
Reactant BRN (.RBRN):	7434131, 4291410
Reactant (.RCT):	6,7,8,9-tetrahydro-4-phenylbenzo<g>phthalazin-1(2H)-one, 1-(2-chloro-ethyl)-1H-imidazole
Product BRN (.PBRN):	8444536
Product (.PRO):	2-(2-imidazol-1-yl-ethyl)-4-phenyl-6,7,8,9-tetrahydro-2H-benzo<g>phthalazin-1-one
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	8533023.1
Reaction Classification (.CL):	Multistage
Yield (.YDT):	70 percent (BRN=8444536)
Nr. of Stages (.SNR):	2
Stage 1	
Reagent (.RGT):	NaH
Solvent (.SOL):	dimethylformamide
Time (.TIM):	1 hour(s)
Temperature (.T):	20 Cel
Reaction Type (.TYP):	deprotonation
Stage 2	
Stage reactant (.SRCT):	1-(2-chloro-ethyl)-1#H!-imidazole
Stage Reactant BRN (.SRBRN):	4291410
Solvent (.SOL):	dimethylformamide
Time (.TIM):	14 hour(s)
Temperature (.T):	70 Cel
Reaction Type (.TYP):	Substitution

Reference(s):

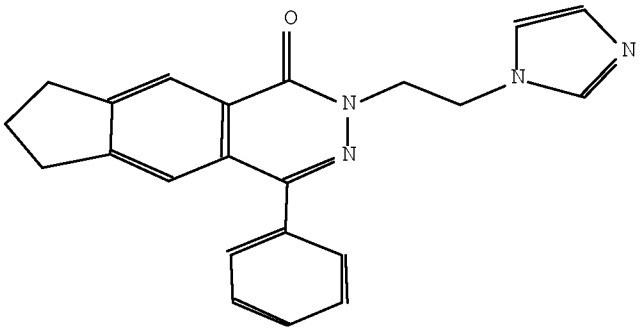
1. Haider, Norbert; Hartmann, Rolf W.; Steinwender, Andreas, Arch.Pharm.(Weinheim Ger.), CODEN: ARPMAS, 332(11), <1999>, 408 - 409; BABS-6205172

=> d ide l39 28

L39 ANSWER 28 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	8441980
Chemical Name (CN):	2,6,7,8-tetrahydro-2-<2-(1-imidazolyl)ethyl>-4-phenyl-1H-cyclopenta<g>phthalazin-1-o

	ne
Autonom Name (AUN):	6-(2-imidazol-1-yl-ethyl)-8-phenyl-1,2,3,6-tetrahydro-6,7-diaza-cyclopenta<b>naphthalen-5-one
Molec. Formula (MF):	C22 H20 N4 O
Molecular Weight (MW):	356.43
Lawson Number (LN):	28744, 28020, 3706
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7162551
Tautomer ID (TAUTID):	7958547
Entry Date (DED):	2000/05/16
Update Date (DUPD):	2000/05/16



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	2
PHARM	Pharmacological Data	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

```
=> d rx l39 28


L39  ANSWER 28 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX
     Reaction ID (.ID):              8532860
     Reactant BRN (.RBRN):           7432249, 4291410
     Reactant (.RCT):                8-phenyl-1,2,3,6-tetrahydro-6,7-diaza-cycl
                                     openta<b>naphthalen-5-one,
                                     1-(2-chloro-ethyl)-1H-imidazole
     Product BRN (.PBRN):            8441980
     Product (.PRO):                 6-(2-imidazol-1-yl-ethyl)-8-phenyl-1,2,3,6
                                     -tetrahydro-6,7-diaza-cyclopenta<b>naphtha
                                     len-5-one
     No. of React. Details (.NVAR):  1

Reaction Details:
RX
     Reaction RID (.RID):            8532860.1
     Reaction Classification (.CL):  Multistage
     Yield (.YDT):                   68 percent (BRN=8441980)
     Nr. of Stages (.SNR):           2
     Stage 1
     Reagent (.RGT):                 NaH
     Solvent (.SOL):                 dimethylformamide
     Time (.TIM):                    1 hour(s)
     Temperature (.T):               20 Cel
     Reaction Type (.TYP):           deprotonation
     Stage 2
     Stage reactant (.SRCT):         1-(2-chloro-ethyl)-1#H!-imidazole
     Stage Reactant BRN (.SRBRN):    4291410
     Solvent (.SOL):                 dimethylformamide
     Time (.TIM):                    14 hour(s)
     Temperature (.T):               70 Cel
     Reaction Type (.TYP):           Substitution
     Reference(s):
     1. Haider, Norbert; Hartmann, Rolf W.; Steinwender, Andreas,
        Arch.Pharm.(Weinheim Ger.), CODEN: ARPMAS, 332(11), <1999>, 408 - 409;
        BABS-6205172


=> d ide l39 29


L39  ANSWER 29 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

     Beilstein Records (BRN):        7434131
     Chemical Name (CN):             6,7,8,9-tetrahydro-4-phenylbenzo<g>phthala
                                     zin-1(2H)-one
     Autonom Name (AUN):             4-phenyl-6,7,8,9-tetrahydro-2H-benzo<g>pht
                                     halazin-1-one
     Molec. Formula (MF):            C18 H16 N2 O
     Molecular Weight (MW):          276.34
     Lawson Number (LN):             28745
     Compound Type (CTYPE):          heterocyclic
     Constitution ID (CONSID):       6358917
     Tautomer ID (TAUTID):           72792
     Beilstein Citation (BSO):       6-24
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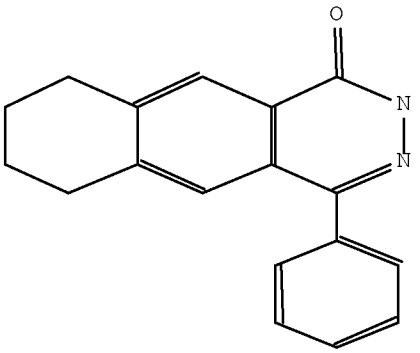
Entry Date (DED): 1996/08/09
Update Date (DUPD): 2000/05/16



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3
RXREA	Substance is Reaction Reactant	2
RXPRO	Substance is Reaction Product	1

=> d rx l39 29

L39 ANSWER 29 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

```
     Reaction ID (.ID):              4417477
     Reactant BRN (.RBRN):           1215280, 114797
     Reactant (.RCT):                4-phenyl-2H-pyridazino<4,5-d>pyridazin-1-o
                                     ne, 1-cyclohex-1-enyl-pyrrolidine
     Product BRN (.PBRN):            7434131
     Product (.PRO):                 6,7,8,9-tetrahydro-4-phenylbenzo<g>phthala
                                     zin-1(2H)-one
     No. of React. Details (.NVAR):  1

Reaction Details:
RX
     Reaction RID (.RID):            4417477.1
     Reaction Classification (.CL):  Preparation
     Reagent (.RGT):                 2.) AcOH
     Other Conditions (.COND):       1.) 1,4-dioxane, reflux, 1 h, 2.)
                                     1-propanol, reflux, 24 h
     Note(s) (.COM):                 Yield given. Multistep reaction
     Reference(s):
     1. Haider, Norbert, Heterocycles, CODEN: HTCYAM, 41(11), <1995>,
        2519-2526; BABS-6008956

Reaction:
RX
     Reaction ID (.ID):              8533023
     Reactant BRN (.RBRN):           7434131, 4291410
     Reactant (.RCT):                6,7,8,9-tetrahydro-4-phenylbenzo<g>phthala
                                     zin-1(2H)-one,
                                     1-(2-chloro-ethyl)-1H-imidazole
     Product BRN (.PBRN):            8444536
     Product (.PRO):                 2-(2-imidazol-1-yl-ethyl)-4-phenyl-6,7,8,9
                                     -tetrahydro-2H-benzo<g>phthalazin-1-one
     No. of React. Details (.NVAR):  1

Reaction Details:
RX
     Reaction RID (.RID):            8533023.1
     Reaction Classification (.CL):  Multistage
     Yield (.YDT):                   70 percent (BRN=8444536)
     Nr. of Stages (.SNR):           2
     Stage 1
     Reagent (.RGT):                 NaH
     Solvent (.SOL):                 dimethylformamide
     Time (.TIM):                    1 hour(s)
     Temperature (.T):               20 Cel
     Reaction Type (.TYP):           deprotonation
     Stage 2
     Stage reactant (.SRCT):         1-(2-chloro-ethyl)-1#H!-imidazole
     Stage Reactant BRN (.SRBRN):    4291410
     Solvent (.SOL):                 dimethylformamide
     Time (.TIM):                    14 hour(s)
     Temperature (.T):               70 Cel
     Reaction Type (.TYP):           Substitution
     Reference(s):
     1. Haider, Norbert; Hartmann, Rolf W.; Steinwender, Andreas,
        Arch.Pharm.(Weinheim Ger.), CODEN: ARPMAS, 332(11), <1999>, 408 - 409;
        BABS-6205172

Reaction:
RX
     Reaction ID (.ID):              4637798
```

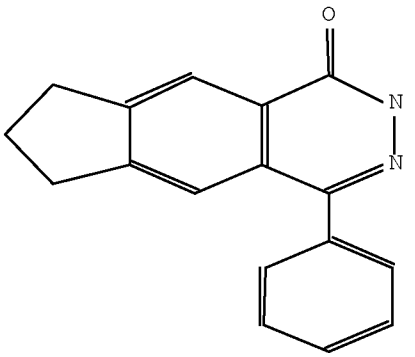
Reactant BRN (.RBRN): 7434131
Reactant (.RCT): 6,7,8,9-tetrahydro-4-phenylbenzo<g>phthalazin-1(2H)-one
Product BRN (.PBRN): 7647989
Product (.PRO): 1-chloro-6,7,8,9-tetrahydro-4-phenylbenzo<g>phthalazine
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 4637798.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 50 percent (BRN=7647989)
Reagent (.RGT): POCl3, N,N-diethylaniline
Time (.TIM): 2 hour(s)
Temperature (.T): 90 Cel
Reference(s):
1. Haider, Norbert; Steinwender, Andreas, Sci.Pharm., CODEN: SCPHA4, 64(3/4), <1996>, 399-406; BABS-6049366

=> d ide l39 30

L39 ANSWER 30 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 7432249
Chemical Name (CN): 2,6,7,8-tetrahydro-4-phenyl-1H-cyclopenta<g>phthalazin-1-one
Autonom Name (AUN): 8-phenyl-1,2,3,6-tetrahydro-6,7-diaza-cyclopenta<b>naphthalen-5-one
Molec. Formula (MF): C17 H14 N2 O
Molecular Weight (MW): 262.31
Lawson Number (LN): 28744
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 6355731
Tautomer ID (TAUTID): 7055539
Beilstein Citation (BSO): 6-24
Entry Date (DED): 1996/08/09
Update Date (DUPD): 2000/05/16



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3
RXREA	Substance is Reaction Reactant	2
RXPRO	Substance is Reaction Product	1

=> d rx l39 30

L39 ANSWER 30 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	4416653
Reactant BRN (.RBRN):	1215280, 109824
Reactant (.RCT):	4-phenyl-2H-pyridazino<4,5-d>pyridazin-1-one, 1-cyclopent-1-enyl-pyrrolidine
Product BRN (.PBRN):	7432249
Product (.PRO):	8-phenyl-1,2,3,6-tetrahydro-6,7-diaza-cyclopenta<b>naphthalen-5-one
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	4416653.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	2.) AcOH
Other Conditions (.COND):	1.) 1,4-dioxane, reflux, 1 h, 2.) 1-propanol, reflux, 24 h
Note(s) (.COM):	Yield given. Multistep reaction

Reference(s):
1. Haider, Norbert, Heterocycles, CODEN: HTCYAM, 41(11), <1995>, 2519-2526; BABS-6008956

Reaction:
RX
Reaction ID (.ID): 8532860
Reactant BRN (.RBRN): 7432249, 4291410
Reactant (.RCT): 8-phenyl-1,2,3,6-tetrahydro-6,7-diaza-cyclopenta<b>naphthalen-5-one, 1-(2-chloro-ethyl)-1H-imidazole
Product BRN (.PBRN): 8441980
Product (.PRO): 6-(2-imidazol-1-yl-ethyl)-8-phenyl-1,2,3,6-tetrahydro-6,7-diaza-cyclopenta<b>naphthalen-5-one
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 8532860.1
Reaction Classification (.CL): Multistage
Yield (.YDT): 68 percent (BRN=8441980)
Nr. of Stages (.SNR): 2
Stage 1
Reagent (.RGT): NaH
Solvent (.SOL): dimethylformamide
Time (.TIM): 1 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): deprotonation
Stage 2
Stage reactant (.SRCT): 1-(2-chloro-ethyl)-1#H!-imidazole
Stage Reactant BRN (.SRBRN): 4291410
Solvent (.SOL): dimethylformamide
Time (.TIM): 14 hour(s)
Temperature (.T): 70 Cel
Reaction Type (.TYP): Substitution
Reference(s):
1. Haider, Norbert; Hartmann, Rolf W.; Steinwender, Andreas, Arch.Pharm.(Weinheim Ger.), CODEN: ARPMAS, 332(11), <1999>, 408 - 409; BABS-6205172

Reaction:
RX
Reaction ID (.ID): 4637784
Reactant BRN (.RBRN): 7432249
Reactant (.RCT): 8-phenyl-1,2,3,6-tetrahydro-6,7-diaza-cyclopenta<b>naphthalen-5-one
Product BRN (.PBRN): 7645601
Product (.PRO): 5-chloro-8-phenyl-2,3-dihydro-1H-6,7-diaza-cyclopenta<b>naphthalene
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 4637784.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 36 percent (BRN=7645601)
Reagent (.RGT): POCl3, N,N-diethylaniline
Time (.TIM): 2 hour(s)
Temperature (.T): 90 Cel
Reference(s):
1. Haider, Norbert; Steinwender, Andreas, Sci.Pharm., CODEN: SCPHA4, 64(3/4), <1996>, 399-406; BABS-6049366

```
=> d ide l39 31

L39  ANSWER 31 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

     Beilstein Records (BRN):        347858
     Chemical Name (CN):             8-(3,4,5-trimethoxy-phenyl)-6H-<1,3>dioxol
                                     o<4,5-g>phthalazin-5-one
     Autonom Name (AUN):             8-(3,4,5-trimethoxy-phenyl)-6H-<1,3>dioxol
                                     o<4,5-g>phthalazin-5-one
     Molec. Formula (MF):            C18 H16 N2 O6
     Molecular Weight (MW):          356.33
     Lawson Number (LN):             32377, 289
     Compound Type (CTYPE):          heterocyclic
     Constitution ID (CONSID):       337329
     Tautomer ID (TAUTID):           359024
     Beilstein Citation (BSO):       4-27-00-08904
     Entry Date (DED):               1988/06/27
     Update Date (DUPD):             1992/05/13
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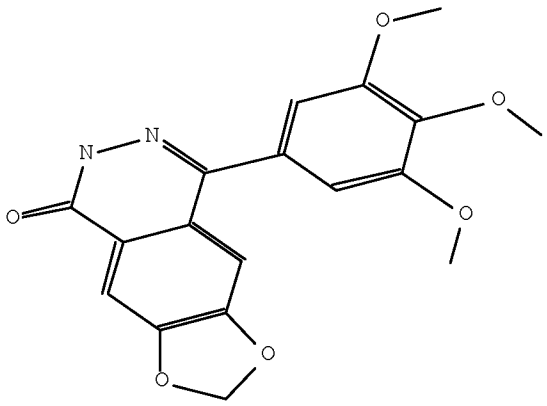

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1

MP	Melting Point	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3
RXREA	Substance is Reaction Reactant	2
RXPRO	Substance is Reaction Product	1

=> d rx l39 31

L39 ANSWER 31 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	5569349
Reactant (.RCT):	6-<3.4.5-trimethoxy-benzoyl>-benzo<1.3>dioxole-5-carboxylic acid
Product BRN (.PBRN):	347858
Product (.PRO):	8-(3,4,5-trimethoxy-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	5569349.1
Reaction Classification (.CL):	Preparation (half reaction)
Reagent (.RGT):	ethanol, N2H4+H2O
Note(s) (.COM):	Handbook

Reference(s):
1. Noguchi; Kawanami, Yakugaku Zasshi, CODEN: YKKZAJ, 60, <1940>, 629, 634, Chem.Abstr., <1953>, 6386

Reaction:
RX

Reaction ID (.ID):	5741896
Reactant BRN (.RBRN):	347858
Reactant (.RCT):	8-(3,4,5-trimethoxy-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
Product (.PRO):	oxime C18H17N3O6
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	5741896.1
Reaction Classification (.CL):	Chemical behaviour (half reaction)
Note(s) (.COM):	Handbook

Reference(s):
1. Noguchi; Kawanami, Yakugaku Zasshi, CODEN: YKKZAJ, 60, <1940>, 629, 634, Chem.Abstr., <1953>, 6386

Reaction:
RX

Reaction ID (.ID):	521344
Reactant BRN (.RBRN):	347858
Reactant (.RCT):	8-(3,4,5-trimethoxy-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one

```
     Product BRN (.PBRN):            355497
     Product (.PRO):                 8-(3,4,5-trimethoxy-phenyl)-6H-<1,3>dioxol
                                     o<4,5-g>phthalazin-5-one oxime
     No. of React. Details (.NVAR):  1

Reaction Details:
RX
     Reaction RID (.RID):            521344.1
     Reaction Classification (.CL):  Preparation
     Note(s) (.COM):                 Handbook
     Reference(s):
     1. Noguchi; Kawanami, Yakugaku Zasshi, CODEN: YKKZAJ, 60, <1940>, 629,
        634, Chem.Abstr., <1953>, 6386


=> d ide l39 32


L39  ANSWER 32 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

     Beilstein Records (BRN):        43230
     Chemical Name (CN):             4-phenyl-2H-naphtho<2,3-g>phthalazine-1,6,
                                     11-trione
     Autonom Name (AUN):             4-phenyl-2H-2,3-diaza-naphthacene-1,6,11-t
                                     rione
     Molec. Formula (MF):            C22 H12 N2 O3
     Molecular Weight (MW):          352.35
     Lawson Number (LN):             28973
     Compound Type (CTYPE):          heterocyclic
     Constitution ID (CONSID):       61454
     Tautomer ID (TAUTID):           82402
     Beilstein Citation (BSO):       4-24-00-02134
     Entry Date (DED):               1988/06/27
     Update Date (DUPD):             1992/05/13
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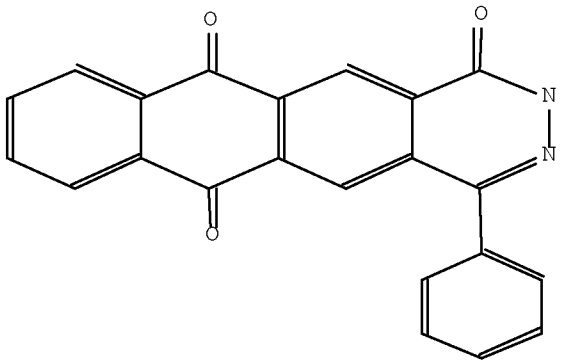


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   Field Availability:

     Code     Name                                   Occurrence
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BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
CPD	Crystal Property Description	1
MP	Melting Point	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d rx l39 32

L39 ANSWER 32 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

Reaction ID (.ID):	514252
Reactant BRN (.RBRN):	3443618
Reactant (.RCT):	3-benzoyl-9,10-dioxo-9,10-dihydro-anthracene-2-carboxylic acid
Product BRN (.PBRN):	43230
Product (.PRO):	4-phenyl-2H-naphtho<2,3-g>phthalazine-1,6,11-trione
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	514252.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	ethanol, N2H4+H2O
Temperature (.T):	120 Cel
Note(s) (.COM):	Handbook

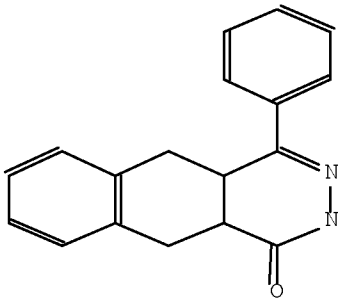
Reference(s):
1. Seka et al., Monatsh.Chem., CODEN: MOCMB7, 57, <1931>, 86,93

=> d ide l39 33

L39 ANSWER 33 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	28738
Beilstein Pref. RN (BPR):	109892-05-9
CAS Reg. No. (RN):	109892-05-9
Chemical Name (CN):	4-phenyl-4a,5,10,10a-tetrahydro-2H-benzo<g

	>phthalazin-1-one
Autonom Name (AUN):	4-phenyl-4a,5,10,10a-tetrahydro-2H-benzo<g
	>phthalazin-1-one
Molec. Formula (MF):	C18 H16 N2 O
Molecular Weight (MW):	276.34
Lawson Number (LN):	28745
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	34762
Tautomer ID (TAUTID):	72792
Beilstein Citation (BSO):	4-24-00-00740
Entry Date (DED):	1988/06/27
Update Date (DUPD):	1992/05/13



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
MP	Melting Point	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

```
=> d rx l39 33


L39  ANSWER 33 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX
     Reaction ID (.ID):              5533353
     Reactant (.RCT):                3-benzoyl-1,2,3,4-tetrahydro-naphthalene-2
                                     -carboxylic acid
     Product BRN (.PBRN):            28738
     Product (.PRO):                 4-phenyl-4a,5,10,10a-tetrahydro-2H-benzo<g
                                     >phthalazin-1-one
     No. of React. Details (.NVAR):  1

Reaction Details:
RX
     Reaction RID (.RID):            5533353.1
     Reaction Classification (.CL):  Preparation (half reaction)
     Reagent (.RGT):                 N2H4+H2O
     Note(s) (.COM):                 Handbook
     Reference(s):
     1. Buchta; Egger, Chem.Ber., CODEN: CHBEAM, 90, <1957>, 2760, 2763
```

```
=> d que nos l30
L1             1 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  US2004-772445/APPS
L8               STR
L10           56 SEA FILE=REGISTRY SSS FUL L8
L13              STR
L15           37 SEA FILE=REGISTRY SUB=L10 SSS FUL L13
L19              QUE  SPE=ON  ABB=ON  PLU=ON  UPASANI, R?/AU
L20              QUE  SPE=ON  ABB=ON  PLU=ON  CAI, S?/AU
L21              QUE  SPE=ON  ABB=ON  PLU=ON  LAN, N?/AU
L22              QUE  SPE=ON  ABB=ON  PLU=ON  WANG, Y?/AU
L23              QUE  SPE=ON  ABB=ON  PLU=ON  FIELD, G?/AU
L24              QUE  SPE=ON  ABB=ON  PLU=ON  FICK, D?/AU
L25              QUE  SPE=ON  ABB=ON  PLU=ON  (COCENSYS OR (PURDUE(1W)PHAR
                 MA) OR (EURO(1W)CELTIQUE))/CS,SO,PA
L27           17 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L15
L28            1 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L27 AND (L19 OR L20
                 OR L21 OR L22 OR L23 OR L24 OR L25)
L29            1 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L1 AND L28
L30            1 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  (L28 OR L29)


=> d his l33

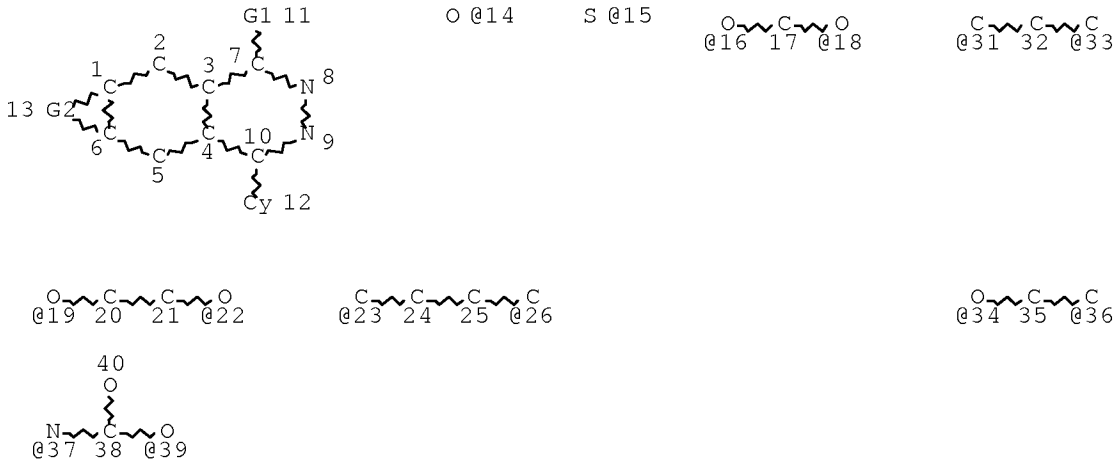
     (FILE 'USPATFULL, USPATOLD, USPAT2, CASREACT, TOXCENTER' ENTERED AT
     15:31:58 ON 04 DEC 2008)
L33            3 S L32 AND L19-L25

=> d que nos l33
L8               STR
L10           56 SEA FILE=REGISTRY SSS FUL L8
L13              STR
L15           37 SEA FILE=REGISTRY SUB=L10 SSS FUL L13
L19              QUE  SPE=ON  ABB=ON  PLU=ON  UPASANI, R?/AU
L20              QUE  SPE=ON  ABB=ON  PLU=ON  CAI, S?/AU
L21              QUE  SPE=ON  ABB=ON  PLU=ON  LAN, N?/AU
L22              QUE  SPE=ON  ABB=ON  PLU=ON  WANG, Y?/AU
L23              QUE  SPE=ON  ABB=ON  PLU=ON  FIELD, G?/AU
L24              QUE  SPE=ON  ABB=ON  PLU=ON  FICK, D?/AU
L25              QUE  SPE=ON  ABB=ON  PLU=ON  (COCENSYS OR (PURDUE(1W)PHAR
                 MA) OR (EURO(1W)CELTIQUE))/CS,SO,PA
L32            9 SEA L15
L33            3 SEA L32 AND (L19 OR L20 OR L21 OR L22 OR L23 OR L24 OR L25)



=> d que nos l42
L13              STR
L19              QUE  SPE=ON  ABB=ON  PLU=ON  UPASANI, R?/AU
L20              QUE  SPE=ON  ABB=ON  PLU=ON  CAI, S?/AU
L21              QUE  SPE=ON  ABB=ON  PLU=ON  LAN, N?/AU
L22              QUE  SPE=ON  ABB=ON  PLU=ON  WANG, Y?/AU
L23              QUE  SPE=ON  ABB=ON  PLU=ON  FIELD, G?/AU
L24              QUE  SPE=ON  ABB=ON  PLU=ON  FICK, D?/AU
L25              QUE  SPE=ON  ABB=ON  PLU=ON  (COCENSYS OR (PURDUE(1W)PHAR
                 MA) OR (EURO(1W)CELTIQUE))/CS,SO,PA
L41            4 SEA FILE=CHEMINFORMRX SSS FUL L13 (     8 REACTIONS)
L42            0 SEA FILE=CHEMINFORMRX SPE=ON  ABB=ON  PLU=ON  L41 AND (L19 OR
                 L20 OR L21 OR L22 OR L23 OR L24 OR L25)
```

```
=> d que l45
L13             STR
```

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VAR G2=16-6 18-1/19-6 22-1/31-6 33-1/23-6 26-1/34-6 36-1/36-6 34-1/37-6 3
9-1/39-6 37-1
NODE ATTRIBUTES:
CONNECT IS E1  RC AT  14
CONNECT IS E1  RC AT  15
CONNECT IS E1  RC AT  40
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT  12
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  36

STEREO ATTRIBUTES: NONE
L45           8 SEA FILE=WPIX SSS FUL L13


=> d que nos l50
L2            1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  US2004-772445/APPS
L13             STR
L19             QUE  SPE=ON  ABB=ON  PLU=ON  UPASANI, R?/AU
L20             QUE  SPE=ON  ABB=ON  PLU=ON  CAI, S?/AU
L21             QUE  SPE=ON  ABB=ON  PLU=ON  LAN, N?/AU
L22             QUE  SPE=ON  ABB=ON  PLU=ON  WANG, Y?/AU
L23             QUE  SPE=ON  ABB=ON  PLU=ON  FIELD, G?/AU
L24             QUE  SPE=ON  ABB=ON  PLU=ON  FICK, D?/AU
L25             QUE  SPE=ON  ABB=ON  PLU=ON  (COCENSYS OR (PURDUE(1W)PHAR
                MA) OR (EURO(1W)CELTIQUE))/CS,SO,PA
L45           8 SEA FILE=WPIX SSS FUL L13
L46           1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  (RA0ON1/DCN OR RA0ON2/DCN
                 OR RA0ON3/DCN OR RA0ON4/DCN OR RA0ON5/DCN OR RA0ON6/DCN OR
                RA0ON7/DCN OR RA0ON8/DCN) OR L45/DCR
L47           1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L46 AND (L19 OR L20 OR
                L21 OR L22 OR L23 OR L24 OR L25)
L49           1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L47 AND L2
```

```
L50           1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L47 OR L49


=> d his l54

     (FILE 'HCAPLUS, WPIX, MEDLINE, BIOSIS, EMBASE, PASCAL, CABA, CEABA-VTB,
     LIFESCI, BIOENG, BIOTECHNO, BIOTECHDS, DRUGU, DRUGB, VETU, VETB,
     SCISEARCH, CONFSCI, DISSABS, RDISCLOSURE' ENTERED AT 15:39:34 ON 04 DEC
     2008)
L54          15 S L52 AND L25

=> d que l54
L19              QUE  SPE=ON  ABB=ON  PLU=ON  UPASANI, R?/AU
L20              QUE  SPE=ON  ABB=ON  PLU=ON  CAI, S?/AU
L21              QUE  SPE=ON  ABB=ON  PLU=ON  LAN, N?/AU
L22              QUE  SPE=ON  ABB=ON  PLU=ON  WANG, Y?/AU
L23              QUE  SPE=ON  ABB=ON  PLU=ON  FIELD, G?/AU
L24              QUE  SPE=ON  ABB=ON  PLU=ON  FICK, D?/AU
L25              QUE  SPE=ON  ABB=ON  PLU=ON  (COCENSYS OR (PURDUE(1W)PHAR
                 MA) OR (EURO(1W)CELTIQUE))/CS,SO,PA
L52          164 SEA (L19 OR L20 OR L21 OR L22 OR L23 OR L24 OR L25) AND
                 ?QUINAZOLIN?/IT,TI,CC,CT,ST,STP
L54           15 SEA L52 AND L25


=> dup rem l30 l33 l42 l50 l54
L42 HAS NO ANSWERS
DUPLICATE IS NOT AVAILABLE IN 'CHEMINFORMRX, RDISCLOSURE'.
ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE
FILE 'HCAPLUS' ENTERED AT 15:58:57 ON 04 DEC 2008
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PROCESSING COMPLETED FOR L30
PROCESSING COMPLETED FOR L33
PROCESSING COMPLETED FOR L42
PROCESSING COMPLETED FOR L50
PROCESSING COMPLETED FOR L54
L56          12 DUP REM L30 L33 L42 L50 L54 (8 DUPLICATES REMOVED)
                ANSWERS '1-6' FROM FILE HCAPLUS
                ANSWERS '7-9' FROM FILE USPATFULL
                ANSWERS '10-11' FROM FILE BIOSIS
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ANSWER '12' FROM FILE SCISEARCH

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=> file stnguide
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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov 21, 2008 (20081121/UP).
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=> d ibib ed abs hitind hitstr 1-6
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, USPATFULL, BIOSIS, SCISEARCH' -
CONTINUE? (Y)/N:y
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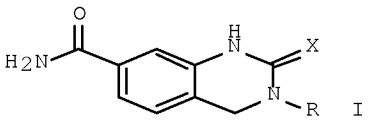
L56 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2004:657939 HCAPLUS Full-text
TITLE: Quinazolinones and benzothiazinones as novel sodium channel blockers
AUTHOR(S): Victory, Sam F.; Sun, Qun; Limberis, Jim; Kyle, Donald J.
CORPORATE SOURCE: Discovery Research, Purdue Pharma, L.P, Cranbury, NJ, 08512, USA
SOURCE: Abstracts of Papers, 228th ACS National Meeting, Philadelphia, PA, United States, August 22-26, 2004 (2004), MEDI-075. American Chemical Society: Washington, D. C.
CODEN: 69FTZ8
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
ED Entered STN: 15 Aug 2004
AB V102862 is a potent state-dependent sodium channel blocker (Ki = 370 nM, rBIIa) that has been shown to be efficacious in the Chung model of neuropathic pain. Toward the discovery of a second-generation compound having an improved pharmaceutical profile, we embarked on a systematic structure-activity investigation aimed at replacing the semicarbazone moiety of V102862 with various heterocycles as a bioisosteric replacement. Our labs. have reported on several series of high affinity sodium channel blockers as part of this effort, including a series of compds. containing a thiazolidinone ring system as a replacement. Some of the most potent compds. in the thiazolidinone series possessed a hydrophobic aryl ether moiety, similar to V102862, and also a piperidinylethylamine moiety. To further explore the bioisosteric replacement of the semicarbazone moiety of V102862, several addnl. series of compds. were synthesized including those having a quinazolin-4(3H)-one or a 2,3-dihydro-benzothiazin-4-one core ring system. Within each of these new series, the optimized piperidinylethylamine group of the thiazolidinone series was held constant while the hydrophobic aryl ether moiety was varied, generating potent sodium channel blockers in each series. Details of the synthesis and SAR of analogs will be presented.

L56 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 2001:420169 HCAPLUS Full-text
DOCUMENT NUMBER: 135:226951
TITLE: Solid-phase synthesis of 3,4-dihydro-2(1H)-quinazolinones and 3,4-dihydro-1H-quinazolin-2-thiones
AUTHOR(S): Sun, Q.; Zhou, X.; Kyle, D. J.
CORPORATE SOURCE: Department of Computational, Combinatorial and Medicinal Chemistry, Purdue Pharma LP, Cranbury, NJ, 08512, USA
SOURCE: Tetrahedron Letters (2001), 42(25), 4119-4121
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:226951

ED Entered STN: 11 Jun 2001
GI



AB Dihydroquinazolinones and dihydroquinazolinethiones I [R = PhCH2, 3-pyridylmethyl, PhCH(Me), 4-MeOC6H4CH2, 4-MeOC6H4CH2CH2, 1-naphthylmethyl, Ph2CHCH2, 1-benzyl-4-piperidinemethyl, 2-(4-morpholinyl)ethyl, Me2NCH2CH2, Me2CHCH2; X = O, S] are prepared on solid phase. E.g., Fmoc-Rink resin was deprotected with piperidine and treated with 4-(bromomethyl)-3-nitrobenzoic acid with 1-hydroxybenzotriazole and diisopropyl carbodiimide to give the resin-bound benzamide; addition of benzylamine gave a resin-bound (benzylaminomethyl)nitrobenzamide which was reduced with tin (II) chloride to give a resin-bound (benzylaminomethyl)aminobenzamide. E.g., treatment of the resin-bound (benzylaminomethyl)aminobenzamide with disuccinimidyl carbonate in DMF followed by cleavage of the resin with trifluoroacetic acid gave the dihydroquinazolinones I (X = O) in 73-100% yields and 60-95% purities, while treatment of the resin-bound (benzylaminomethyl)aminobenzamide with thiocarbonyldiimidazole followed by cleavage of the resin with trifluoroacetic acid gave the dihydroquinazolinethiones I (X = S) in 72-97% yields and 60-89% purities.

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

ST hydroquinazolinone hydroquinazolinethione solid phase prepn; quinazolinone quinazolinethione solid phase prepn

IT Solid phase synthesis
(solid-phase preparation of substituted quinazolinones and quinazolinethiones)

IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(solid-phase preparation of substituted quinazolinones and quinazolinethiones)

IT 55-81-2, 4-Methoxyphenethyl amine 78-81-9, Isobutylamine 100-46-9, Benzylamine, reactions 108-00-9, 2-(Dimethylamino)ethylamine 118-31-0, 1-Naphthylmethylamine 618-36-0, α-Methylbenzylamine 2038-03-1, 2-(4-Morpholinyl)ethylamine 2393-23-9, 4-Methoxybenzylamine 3731-52-0, 3-Pyridylmethylamine 5586-73-2, 3,3-Diphenylpropylamine 50541-93-0 55715-03-2D, 3-Nitro-4-(bromomethyl)benzoic acid, resin-bound 84418-43-9D, resin-bound
RL: RCT (Reactant); RACT (Reactant or reagent)
(solid-phase preparation of substituted quinazolinones and quinazolinethiones)

IT 358718-76-0P 358718-77-1P 358718-78-2P 358718-79-3P 358718-80-6P 358718-81-7P 358718-82-8P 358718-83-9P 358718-84-0P 358718-85-1P 358718-86-2P 358718-87-3P 358718-88-4P 358718-89-5P 358718-90-8P 358718-91-9P 358718-92-0P 358718-93-1P 358718-94-2P 358718-95-3P 358718-96-4P 358718-97-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid-phase preparation of substituted quinazolinones and quinazolinethiones)

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

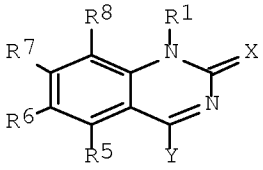
L56 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 1999:576785 HCAPLUS Full-text
DOCUMENT NUMBER: 131:214294
TITLE: Preparation of substituted quinazolines and heterocyclic analogs as antagonists or positive modulators of AMPA receptors
INVENTOR(S): Opasani, Ravi; Cai, Sui X.; Lan, Nancy C.; Wang, Yan; Field, George; Fick, David B.
PATENT ASSIGNEE(S): Cocensys, Inc., USA
SOURCE: PCT Int. Appl., 117 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9944612	A1	19990910	WO 1999-US4609	19990302
W: JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1066039	A1	20010110	EP 1999-911063	19990302
R: BE, CH, DE, ES, FR, GB, IT, LI, NL, IE				
JP 2002505288	T	20020219	JP 2000-534214	19990302
US 6465472	B1	20021015	US 2000-654839	20000901
US 20030033089	A1	20030213	US 2002-219755	20020816
US 6765006	B2	20040720		
US 20040162299	A1	20040819	US 2004-772445	20040206 <--

PRIORITY APPLN. INFO.:

US 1998-76451P	P	19980302
WO 1999-US4609	W	19990302
US 2000-654839	A3	20000901
US 2002-219755	A3	20020816

OTHER SOURCE(S): MARPAT 131:214294
ED Entered STN: 14 Sep 1999
GI



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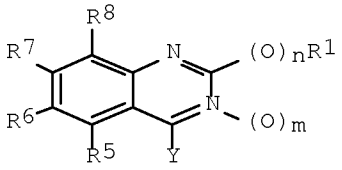

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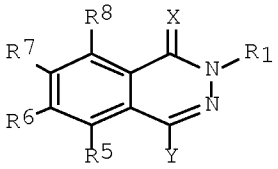

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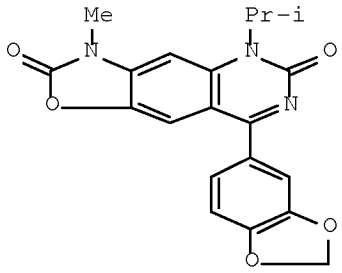


IV

AB Substituted quinazolines and heterocyclic analogs (I, II, and III) [R1 = (un)substituted alkyl, alkenyl, or alkynyl; R5 and R8 = independently H, halogen, NO2, NH2, CN, alkanoylamido, OH, SH, alkoxy, (un)substituted alkyl, (hetero)aryl, heterocyclic, alkenyl, or alkynyl, etc.; R6 and R7 taken together = 5- or 6-membered carbocyclic or heterocyclic ring; X = O or S; Y = (hetero)aryl; n and m = independently 0 or 1] were prepared as antagonists or pos. modulators of AMPA receptors for treatment, prevention, or amelioration of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia. Thus, 3-methyl-5-nitro-2(3H)-benzoxazolone was reduced to the amine over Pt/C in glacial acetic acid. Na cyanoborohydride was added to a suspension of the amine, THF, acetic acid, and acetone followed by treatment with NaOH and water to precipitate 5-(isopropylamino)-3-methyl-2(3H)-benzoxazolone. The substituted amine was converted to the ureido derivative by stirring with KCNO in glacial acetic acid for 5 days. The urea was cyclized with piperonal in benzene and methanesulfonic acid to form the 3,4-dihydrooxazolo[4,5-g]quinazolin-2(1H)-one. The product was reduced by addition of KMnO4 in H2O followed by treatment with formalin to yield 1-isopropyl-4-(3,4-methylenedioxyphenyl)-8-methyl-7-oxooxazolo[4,5-g]quinazolin-2(1H)-one (IV). Selected compds. of the invention were tested for preferred binding to AMPA receptors and exhibited IC50 values ranging from 0.2 to 13 μM. The anticonvulsant activity of the AMPA antagonists was evaluated in the Maximal Electroshock-induced Seizure (MES) test. MES ED50 values ranged from 1 to 10 mg/kg i.v.

IC ICM A61K031-50
ICS A61K031-505; C07D237-26; C07D239-70; C07D491-04; C07D491-048; C07D491-056; C07D498-04

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

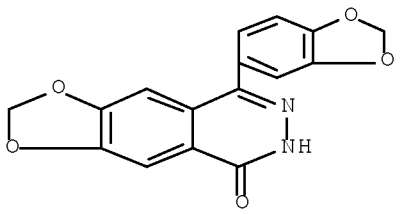
IT 10368-14-6P 33095-75-9P 33095-79-3P 33095-82-8P 33095-94-2P
34060-22-5P 40484-04-6P 59856-06-3P 63546-19-0P 85575-57-1P
164526-15-2P 243133-76-8P 243133-77-9P 243133-78-0P 243133-79-1P
243133-81-5P 243133-82-6P 243133-85-9P 243133-86-0P 243133-88-2P
243133-90-6P 243133-92-8P 243133-94-0P 243133-95-1P 243133-96-2P
243133-97-3P 243133-98-4P 243133-99-5P 243134-07-8P 243134-13-6P
243134-40-9P 243134-48-7P 243134-49-8P 243134-53-4P 243134-58-9P
243134-66-9P 243134-73-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

IT 13067-19-1P 33095-76-0P 33100-29-7P 40483-99-6P 119179-46-3P
243133-80-4P 243133-83-7P 243133-84-8P 243133-87-1P 243133-89-3P
243133-91-7P 243133-93-9P 243134-00-1P 243134-01-2P 243134-02-3P
243134-03-4P 243134-04-5P 243134-05-6P 243134-06-7P 243134-08-9P
243134-09-0P 243134-10-3P 243134-11-4P 243134-12-5P 243134-14-7P
243134-15-8P 243134-16-9P 243134-17-0P 243134-18-1P 243134-19-2P
243134-20-5P 243134-21-6P 243134-22-7P 243134-23-8P 243134-24-9P
243134-25-0P 243134-26-1P 243134-27-2P 243134-28-3P 243134-29-4P
243134-30-7P 243134-31-8P 243134-32-9P 243134-33-0P 243134-34-1P
243134-35-2P 243134-36-3P 243134-37-4P 243134-38-5P 243134-42-1P
243134-44-3P 243134-46-5P 243134-50-1P 243134-51-2P 243134-52-3P
243134-54-5P 243134-55-6P 243134-56-7P 243134-57-8P 243134-59-0P
243134-60-3P 243134-61-4P 243134-62-5P 243134-63-6P 243134-64-7P
243134-65-8P 243134-67-0P 243134-68-1P
243134-69-2P 243134-70-5P 243134-71-6P
243134-72-7P 243134-74-9P 243134-75-0P 243134-76-1P
243134-77-2P 243134-78-3P 243134-79-4P 243134-80-7P 243134-81-8P
243134-82-9P 243134-83-0P 243134-84-1P 243134-85-2P 243134-86-3P
243134-87-4P 243134-88-5P 243134-89-6P 243134-90-9P 243134-91-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

IT 243134-66-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

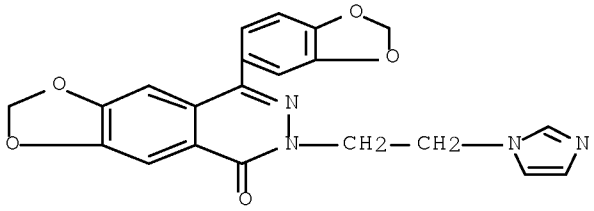
RN 243134-66-9 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)- (CA INDEX NAME)



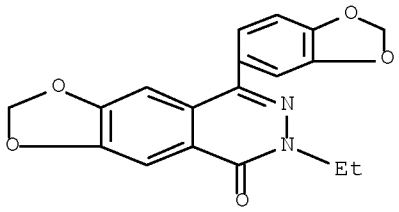
IT 243134-67-0P 243134-68-1P 243134-69-2P
243134-70-5P 243134-71-6P 243134-72-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

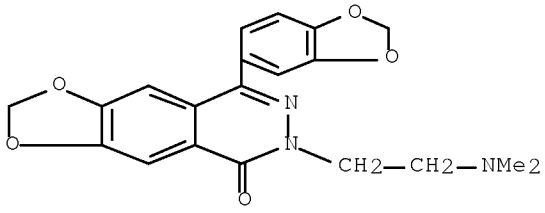
RN 243134-67-0 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)-6-[2-(1H-imidazol-1-yl)ethyl]- (CA INDEX NAME)



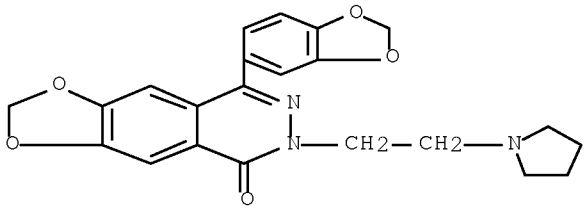
RN 243134-68-1 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)-6-ethyl- (CA INDEX NAME)



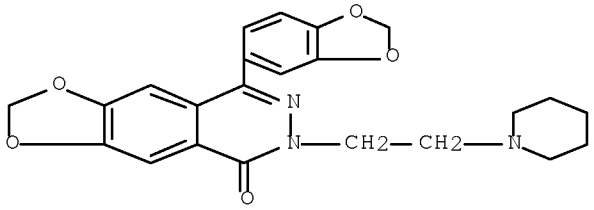
RN 243134-69-2 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)-6-[2-(dimethylamino)ethyl]- (CA INDEX NAME)



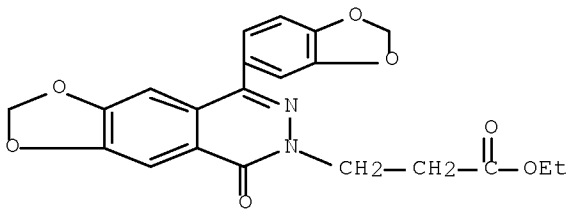
RN 243134-70-5 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)-6-[2-(1-pyrrolidinyl)ethyl]- (CA INDEX NAME)



RN 243134-71-6 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 243134-72-7 HCAPLUS
CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-propanoic acid,
8-(1,3-benzodioxol-5-yl)-5-oxo-, ethyl ester (CA INDEX NAME)



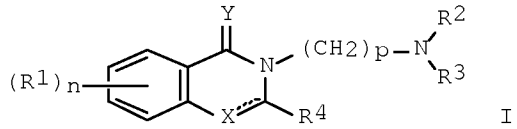
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L56 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:120836 HCAPLUS Full-text
DOCUMENT NUMBER: 140:181460
TITLE: Preparation of (piperidinylethyl)benzoheterocyclic compounds for use as sodium channel blockers
INVENTOR(S): Sun, Qun; Kyle, Donald J.; Victory, Samuel F.
PATENT ASSIGNEE(S): Euro-Celtique S.A., Luxembourg
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004013111	A1	20040212	WO 2003-US23791	20030730
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20040152696	A1	20040805	US 2003-628487	20030729
CA 2493737	A1	20040212	CA 2003-2493737	20030730
AU 2003257015	A1	20040223	AU 2003-257015	20030730
EP 1534690	A1	20050601	EP 2003-766980	20030730
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003013369	A	20050621	BR 2003-13369	20030730
CN 1678592	A	20051005	CN 2003-820742	20030730
JP 2006500343	T	20060105	JP 2004-526225	20030730
MX 2005PA01288	A	20050908	MX 2005-PA1288	20050201
IN 2005KN00293	A	20051125	IN 2005-KN293	20050228
PRIORITY APPLN. INFO.:			US 2002-399702P P	20020801
			WO 2003-US23791 W	20030730

OTHER SOURCE(S): MARPAT 140:181460
ED Entered STN: 13 Feb 2004
GI



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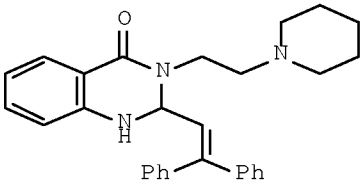

II

AB Title compds. I [wherein R1 = independently halogen, (halo)alkyl, alkoxy, hydroxyalkyl, amino, nitro, cyano; R2, R3 = independently H, (cyclo)alkyl, haloalkyl, hydroxyalkyl, or R2 and R3 together with the nitrogen atom to which they are attached form an (un)substituted heterocyclic ring; R4 = (un)substituted phenoxyphenyl, phenylthiophenyl, phenylaminophenyl, benzylphenyl, etc.; n = 0-3; p = 2-4; X = N, NH, S; Y = O, S; and pharmaceutically acceptable salts or solvates thereof] were prepared as sodium channel blockers. For example, reaction of 2-(piperidin-1-yl)ethylamine with

2-nitrobenzoyl chloride, followed by 10% Pd/C-catalyzed reduction and condensation with 3,3-diphenylpropenal, gave II. I were formulated as tablets and i.v. solns. Selected compds. of the invention inhibited sodium channel activity with Ki values ranging from 1 nM to 3960 nM. Thus, I and their pharmaceutical compns. are useful as sodium channel blockers for the treatment of neuronal damage following global or focal ischemia, neurodegenerative conditions, such as amyotrophic lateral sclerosis (ALS), acute or chronic pain, neuropathic pain, surgical pain, tinnitus, convulsions, manic depression, arrhythmia and diabetic neuropathy (no data).

IC ICM C07D239-91
ICS C07D279-08; A61K031-517; A61K031-5415

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

ST quinazolinone piperidinylethyl prepn sodium channel blocker; benzothiazinone piperidinylethyl prepn sodium channel blocker; benzoheterocycle piperidinylethyl prepn antiischemic analgesics antidepressant antiarrhythmics antitinnitus anticonvulsants

IT Pain
(acute; preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

IT Nervous system, disease
(amyotrophic lateral sclerosis; preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

IT Heart, disease
(arrhythmia; preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

IT Pain
(chronic; preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

IT Nerve, disease
Nervous system, disease
(degeneration; preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

IT Mental and behavioral disorders
(depression, manic; preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

IT Nerve, disease
(diabetic neuropathy; preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

IT Anesthetics
(local; preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

IT Antidepressants
(manic; preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

IT Nerve, disease
Pain
(neuralgia; preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

IT Cytoprotective agents
Nervous system agents
(neuroprotective agents; preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

IT Analgesics
Anti-ischemic agents
Antiarrhythmics
Anticonvulsants
Convulsion

Human
Ischemia
Sodium channel blockers
Tinnitus
(preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

IT Drug delivery systems
(solns., i.v.; preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

IT Pain
(surgical; preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

IT Drug delivery systems
(tablets; preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

IT 658044-66-7P 658044-67-8P 658044-68-9P 658044-69-0P 658044-70-3P
658044-71-4P 658044-72-5P 658044-73-6P 658044-74-7P 658044-75-8P
658044-77-0P 658044-79-2P 658044-81-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

IT 84-58-2, 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone 147-93-3, 2-Mercaptobenzoic acid 610-14-0, 2-Nitrobenzoyl chloride 1074-01-7, Benzoic acid, o-mercaptothio- 1210-39-5 1700-37-4, 3-Benzyloxybenzaldehyde 27578-60-5, 2-(Piperidin-1-yl)ethylamine 69770-23-6 78725-46-9 79124-76-8, 3-(3,4-Dichlorophenoxy)benzaldehyde 137736-06-2, 4-(4-Fluorophenoxy)benzaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

L56 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:635488 HCAPLUS Full-text
TITLE: A facile thermal conversion of arylcyanoguanidines to 2,4-diaminoquinazolines
AUTHOR(S): Shao, Bin; Huang, Jin-cheng
CORPORATE SOURCE: Computational, Combinatorial and Medicinal Chemistry department, Purdue Pharma, L.P, Cranbury, NJ, 08512, USA
SOURCE: Abstracts of Papers, 226th ACS National Meeting, New York, NY, United States, September 7-11, 2003 (2003), ORGN-401. American Chemical Society: Washington, D. C.
CODEN: 69EKY9
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
ED Entered STN: 15 Aug 2003
AB Herein we would like to report a facile, thermally induced conversion of arylcyanoguanidines to 2,4-diaminoquinazolines. Diphenoxycyanoimidate was sequentially treated with anilines of diverse electronic properties followed by secondary amines to form stable intermediates of type B, which upon heating at 120°C in p-xylene in the absence of catalyst cyclize to give high yields of 2,4-diaminoquinazolines (Scheme 1).

L56 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:503392 HCAPLUS Full-text
DOCUMENT NUMBER: 127:149079

ORIGINAL REFERENCE NO.: 127:28801a,28804a
TITLE: Preparation of 4-substituted piperidine analogs and their use as subtype selective NMDA receptor antagonists
INVENTOR(S): Bigge, Christopher F.; Cai, Sui Xiong; Weber, Eckard; Woodward, Richard; Keana, John F. W.; Lan, Nancy C.; Guzikowski, Anthony P.; Zhou, Zhang-Lin; Yeun, Po-Wai
PATENT ASSIGNEE(S): Warner-Lambert Company, USA; Cocensys, Inc.; Bigge, Christopher F.; Cai, Sui Xiong; Weber, Eckard; Woodward, Richard; Keana, John F. W.; Lan, Nancy C.; Guzikowski, Anthony P.; et al.
SOURCE: PCT Int. Appl., 280 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9723216	A1	19970703	WO 1996-US20872		19961220
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN					
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
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CA 2240275	A1	19970703	CA 1996-2240275		19961220
AU 9716899	A	19970717	AU 1997-16899		19961220
AU 717185	B2	20000316			
EP 869792	A2	19981014	EP 1996-945682		19961220
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
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HU 9901296	A3	20010129			
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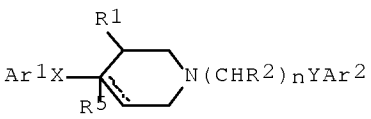
NZ 330624	A	20000327	NZ 1996-330624		19961220
IL 125061	A	20040512	IL 1996-125061		19961220
AT 290380	T	20050315	AT 1996-945682		19961220
NO 9802870	A	19980824	NO 1998-2870		19980619
NO 314580	B1	20030414			
BG 63380	B1	20011231	BG 1998-102562		19980619
US 6124323	A	20000926	US 1998-91598		19980916
PRIORITY APPLN. INFO.:			US 1995-9184P	P	19951222
			WO 1996-US20872	W	19961220

OTHER SOURCE(S): MARPAT 127:149079
ED Entered STN: 09 Aug 1997
GI



I

AB 4-Substituted piperidine analogs I [Ar1, Ar2 = aryl, heteroaryl; X = (CHR3)m, O, S, NR4; R3 = H, OH, alkyl; R4 = H, alkyl; m = 0, 1, 2; R1 = H, OH, alkyl; n = 0-4; Y = O, S, NR4, or a single bond; R5 = H, OH; the dotted bond is a single or double bond] were prepared as selective active antagonists of N-methyl-D-aspartate (NMDA) receptor subtypes. E.g., reaction of 4-benzylpiperidine and 1-bromo-2-phenoxyethane gave 4-benzyl-1-(2-phenoxyethyl)piperidine. Data show that I exhibit selectivity for 2B subtype receptors compared to 2A and 2C subtype receptors. Many of the compds. are active as anticonvulsants. I also show significant protection from ischemia.

IC ICM A61K031-445
ICS C07D211-14

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63

IT 88-75-5, 2-Nitrophenol 90-15-3, 1-Naphthyl alcohol 98-17-9, 3-(Trifluoromethyl)phenol 100-02-7, reactions 100-39-0, Benzyl bromide 100-48-1, 4-Cyanopyridine 100-61-8, N-Methylaniline, reactions 100-83-4, 3-Hydroxybenzaldehyde 103-16-2, 4-Benzyloxyphenol 103-63-9, (2-Bromoethyl)benzene 104-81-4, 4-Methylbenzyl bromide 104-82-5, 4-Methylbenzyl chloride 106-47-8, 4-Chloroaniline, reactions 106-89-8, reactions 108-95-2, Phenol, reactions 108-98-5, Thiophenol, reactions 109-04-6, 2-Bromopyridine 148-24-3, 8-Hydroxyquinoline, reactions 332-48-9 367-12-4, 2-Fluorophenol 371-40-4, 4-Fluoroaniline 371-41-5, 4-Fluorophenol 402-49-3, 4-(Trifluoromethyl)benzyl bromide 452-74-4 459-46-1, 4-Fluorobenzyl bromide 462-06-6, Fluorobenzene 491-36-1, 4-Hydroxyquinazoline 498-94-2, Isonipecotic acid 501-97-3 533-31-3, Sesamol 536-60-7, 4-Isopropylbenzyl alcohol 554-84-7, 3-Nitrophenol 580-13-2, 2-Bromonaphthalene 580-16-5, 6-Hydroxyquinoline 588-63-6 589-10-6, 1-Bromo-2-phenoxyethane 603-35-0, Triphenylphosphine, reactions 603-85-0, 2-Amino-3-nitrophenol 610-81-1, 4-Amino-3-nitrophenol 621-37-4, 3-Hydroxyphenylacetic acid 621-87-4, Phenoxyacetone 622-08-2, 2-Benzyloxyethanol 637-59-2, 1-Bromo-3-phenylpropane 637-89-8, 4-Hydroxythiophenol 768-56-9, 4-Phenyl-1-butene 771-99-3, 4-Phenylpiperidine 876-02-8 877-65-6, 4-tert-Butylbenzyl alcohol 1072-85-1 1129-78-8 1190-22-3, 1,3-Dichlorobutane 1200-03-9, 4-Phenoxybutyl bromide 1476-11-5 1936-57-8, 4-Methylaminophenol sulfate 2033-76-3 2041-17-0 2042-14-0, 4-Methyl-3-nitrophenol 2116-65-6, 4-Benzylpyridine 3245-45-2 3351-59-5 3384-04-1, 3-Phenoxypropyl chloride 3612-20-2 4409-11-4 4463-59-6 4783-86-2, 4-Phenoxypyridine 4830-93-7, 1-Chloro-4-phenylbutane 6748-48-7 6940-76-7, 1-Chloro-3-iodopropane 10315-03-4 13288-06-7 13633-25-5, 1-Bromo-4-phenylbutane 17138-28-2, Ethyl 4-Hydroxyphenylacetate 18800-34-5 18800-37-8 19524-06-2, 4-Bromopyridine hydrochloride 20662-53-7 22009-38-7, 7-Hydroxy-1-tetralone 22921-76-2 31252-42-3, 4-Benzylpiperidine 31406-95-8 33349-49-4 34361-23-4 36938-76-8 36968-94-2 37142-39-5 37581-26-3 39512-49-7 39546-32-2, Isonipecotamide 40807-61-2 41979-39-9, 4-Piperidone hydrochloride 43224-81-3, 2-Phenoxyethyl tosylate 50562-02-2 51135-96-7, 4-Benzyl-4-hydroxypiperidine 51304-58-6 51974-48-2 57825-30-6, 4-Ethylbenzyl bromide 59216-77-2 70743-66-7 79098-85-4 85118-00-9, 2,6-Difluorobenzyl bromide 85118-01-0, 3,4-Difluorobenzyl bromide 92822-01-0 92822-03-2 107332-83-2 118495-07-1 141498-79-5 152604-19-8 177172-38-2 192182-59-5 192872-94-9 192872-97-2 193220-23-4 193356-97-7 193356-99-9 193357-07-2 193357-11-8 193357-17-4 193357-21-0 193357-26-5 193357-31-2 193357-34-5 193357-36-7 193357-39-0 193357-42-5 193357-43-6 193357-44-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of piperidine derivs. and their use as subtype selective NMDA receptor antagonists)

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YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, USPATFULL, BIOSIS, SCISEARCH' -
CONTINUE? (Y)/N:y

L56 ANSWER 7 OF 12 USPATFULL on STN DUPLICATE 3
ACCESSION NUMBER: 2002:268763 USPATFULL Full-text
TITLE: Substituted quinazolines and analogs and use thereof
INVENTOR(S): Upasani, Ravi, San Jose, CA, United States
Cai, Sui X., San Diego, CA, United States
Lan, Nancy C., S. Pasadena, CA, United States
Wang, Yan, San Diego, CA, United States
Field, George, Danville, CA, United States
Fick, David B., Newport Beach, CA, United States
PATENT ASSIGNEE(S): Euro-Celtique S.A., Luxembourg, LUXEMBOURG (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6465472	B1	20021015
APPLICATION INFO.:	US 2000-654839		20000901 (9)

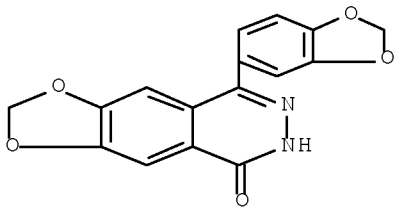
RELATED APPLN. INFO.: Continuation of Ser. No. WO 1999-US4609, filed on 2 Mar 1999

	NUMBER	DATE
PRIORITY INFORMATION:	US 1998-76451P	19980302 (60)

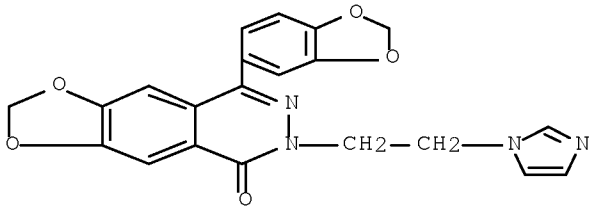
DOCUMENT TYPE: Utility
FILE SEGMENT: GRANTED
PRIMARY EXAMINER: Shah, Mukund J.
ASSISTANT EXAMINER: Liu, Hong
LEGAL REPRESENTATIVE: Sterne, Kessler, Goldstein & Fox P.L.L.C.
NUMBER OF CLAIMS: 16
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 0 Drawing Figure(s); 0 Drawing Page(s)
LINE COUNT: 2866
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention relates to novel quinazolines and heterocycles which are antagonists or positive modulators of AMPA receptors, and the use thereof for treating, preventing or ameliorating neuronal loss associated with stroke, global and focal ischemia, CNS trauma, hypoglycemia and surgery, as well as treating or ameliorating neurodegenerative diseases including Alzheimer's disease, amyotrophic lateral sclerosis, Huntington's disease, Parkinson's disease and Down's syndrome, treating, preventing or ameliorating the adverse consequences of the overstimulation of the excitatory amino acids, treating, preventing or ameliorating anxiety, psychosis, convulsions, chronic pain, glaucoma, retinitis, urinary incontinence, muscular spasm and inducing anesthesia, as well as for treating or ameliorating the adverse consequences of excitatory amino acid deficiency such as schizophrenia, myoclonus. Alzheimer's disease and malnutrition and neural maldevelopment, and as cognition and learning enhancers.

IT 243134-66-9P
(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)
RN 243134-66-9 USPATFULL
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)- (CA INDEX NAME)



IT 243134-67-0P 243134-68-1P 243134-69-2P
243134-70-5P 243134-71-6P 243134-72-7P
(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)
RN 243134-67-0 USPATFULL
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)-6-[2-(1H-imidazol-1-yl)ethyl]- (CA INDEX NAME)



RN 243134-68-1 USPATFULL
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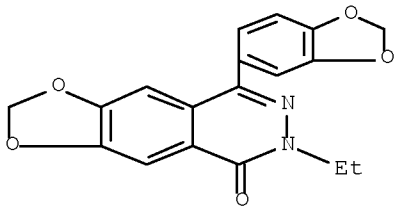

RN 243134-69-2 USPATFULL
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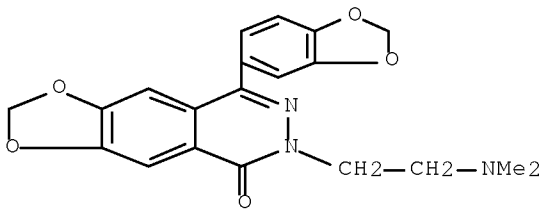
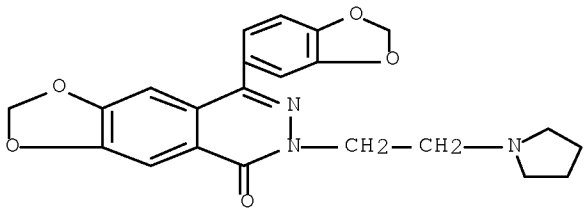
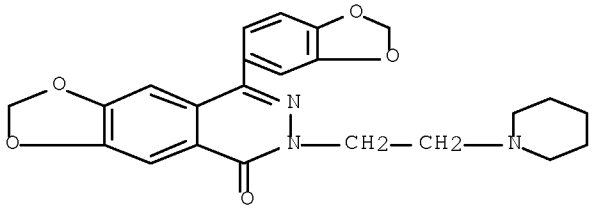
8-(1,3-benzodioxol-5-yl)-6-[2-(dimethylamino)ethyl]- (CA INDEX NAME)



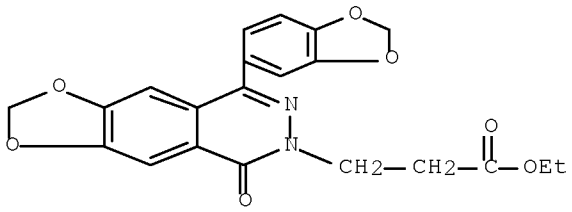
RN 243134-70-5 USPATFULL
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(1-pyrrolidinyl)ethyl]- (CA INDEX NAME)



RN 243134-71-6 USPATFULL
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 243134-72-7 USPATFULL
CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-propanoic acid,
8-(1,3-benzodioxol-5-yl)-5-oxo-, ethyl ester (CA INDEX NAME)



L56 ANSWER 8 OF 12 USPATFULL on STN

ACCESSION NUMBER:	2004:209865 USPATFULL Full-text
TITLE:	Substituted quinazolines and analogs and the use thereof
INVENTOR(S):	Upasani, Ravi, San Jose, CA, UNITED STATES Cai, Sui X., San Diego, CA, UNITED STATES Lan, Nancy C., Pasadena, CA, UNITED STATES Wang, Yan, San Diego, CA, UNITED STATES Field, George, Danville, CA, UNITED STATES Fick, David B., Mission Viejo, CA, UNITED STATES
PATENT ASSIGNEE(S):	Euro-Celtique, S.A. (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 20040162299	A1	20040819
APPLICATION INFO.:	US 2004-772445	A1	20040206 (10)

RELATED APPLN. INFO.: Division of Ser. No. US 2002-219755, filed on 16 Aug 2002, PENDING Division of Ser. No. US 2000-654839, filed on 1 Sep 2000, GRANTED, Pat. No. US 6465472 Continuation of Ser. No. WO 1999-US4609, filed on 2 Mar 1999, PENDING

	NUMBER	DATE
PRIORITY INFORMATION:	US 1998-76451P	19980302 (60)

DOCUMENT TYPE:	Utility
FILE SEGMENT:	APPLICATION
LEGAL REPRESENTATIVE:	STERNE, KESSLER, GOLDSTEIN & FOX PLLC, 1100 NEW YORK AVENUE, N.W., WASHINGTON, DC, 20005
NUMBER OF CLAIMS:	33
EXEMPLARY CLAIM:	1
LINE COUNT:	3033

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention relates to novel quinazolines and heterocycles which are antagonists or positive modulators of AMPA receptors, and the use thereof for treating, preventing or ameliorating neuronal loss associated with stroke, global and focal ischemia, CNS trauma, hypoglycemia and surgery, as well as treating or ameliorating neurodegenerative diseases including Alzheimer's disease, amyotrophic lateral sclerosis, Huntington's disease, Parkinson's disease and Down's syndrome, treating, preventing or ameliorating the adverse consequences of the overstimulation of the excitatory amino acids, treating, preventing or ameliorating anxiety, psychosis, convulsions, chronic pain, glaucoma, retinitis, urinary incontinence, muscular spasm and inducing anesthesia, as well as for treating or ameliorating the adverse consequences of excitatory amino acid

deficiency such as schizophrenia, myoclonus, Alzheimer's disease and malnutrition and neural maldevelopment, and as cognition and learning enhancers.

IT 243134-66-9P

(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

RN 243134-66-9 USPATFULL

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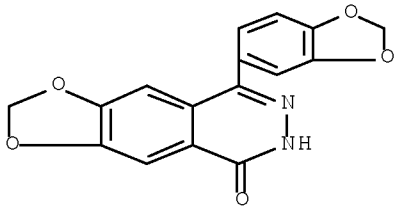
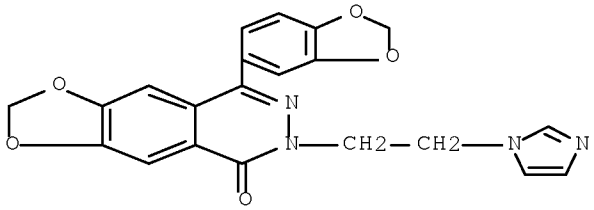


IT 243134-67-0P 243134-68-1P 243134-69-2P
243134-70-5P 243134-71-6P 243134-72-7P

(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

RN 243134-67-0 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)-6-[2-(1H-imidazol-1-yl)ethyl]- (CA INDEX NAME)



RN 243134-68-1 USPATFULL

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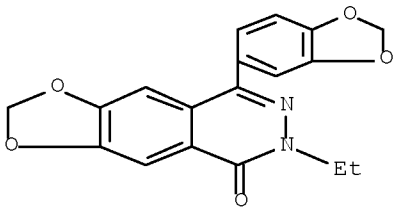
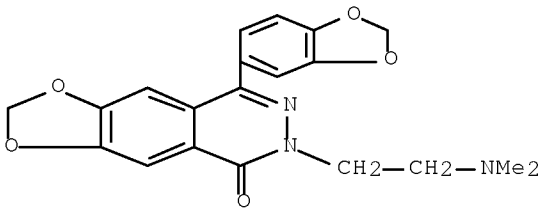
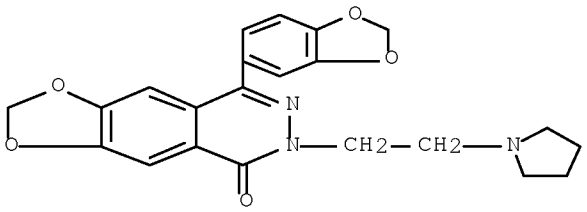


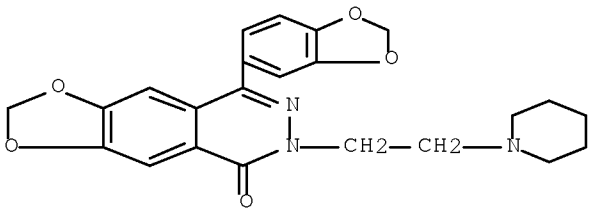
RN 243134-69-2 USPATFULL
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(dimethylamino)ethyl]- (CA INDEX NAME)



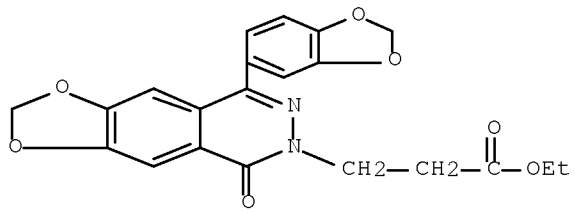
RN 243134-70-5 USPATFULL
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(1-pyrrolidinyl)ethyl]- (CA INDEX NAME)



RN 243134-71-6 USPATFULL
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 243134-72-7 USPATFULL
CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-propanoic acid, 8-(1,3-benzodioxol-5-yl)-5-oxo-, ethyl ester (CA INDEX NAME)



L56 ANSWER 9 OF 12 USPATFULL on STN

ACCESSION NUMBER:	2003:45776 USPATFULL Full-text
TITLE:	Substituted quinazolines and analogs and the use thereof
INVENTOR(S):	Upasani, Ravi, Sunnyvale, CA, UNITED STATES Cai, Sui X., San Diego, CA, UNITED STATES Lan, Nancy C., Altadena, CA, UNITED STATES
PATENT ASSIGNEE(S):	Euro-Celtique S.A. (U.S. corporation)

PATENT INFORMATION:	NUMBER	KIND	DATE
	US 20030033089	A1	20030213
	US 6765006	B2	20040720
APPLICATION INFO.:	US 2002-219755	A1	20020816 (10)

RELATED APPLN. INFO.: Division of Ser. No. US 2000-654839, filed on 1 Sep 2000, GRANTED, Pat. No. US 6465472 Continuation of Ser. No. WO 1999-US4609, filed on 2 Mar 1999, PENDING

PRIORITY INFORMATION:	NUMBER	DATE
	US 1998-76451P	19980302 (60)

DOCUMENT TYPE:	Utility
FILE SEGMENT:	APPLICATION
LEGAL REPRESENTATIVE:	STERNE, KESSLER, GOLDSTEIN & FOX PLLC, 1100 NEW YORK AVENUE, N.W., SUITE 600, WASHINGTON, DC, 20005-3934
NUMBER OF CLAIMS:	33
EXEMPLARY CLAIM:	1
LINE COUNT:	3018

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention relates to novel quinazolines and heterocycles which are antagonists or positive modulators of AMPA receptors, and the use thereof for treating, preventing or ameliorating neuronal loss associated with stroke, global and focal ischemia, CNS trauma, hypoglycemia and surgery, as well as treating or ameliorating neurodegenerative diseases including Alzheimer's disease, amyotrophic lateral sclerosis, Huntington's disease, Parkinson's disease and Down's syndrome, treating, preventing or ameliorating the adverse consequences of the overstimulation of the excitatory amino acids, treating, preventing or ameliorating anxiety, psychosis, convulsions, chronic pain, glaucoma, retinitis, urinary incontinence, muscular spasm and inducing anesthesia, as well as for

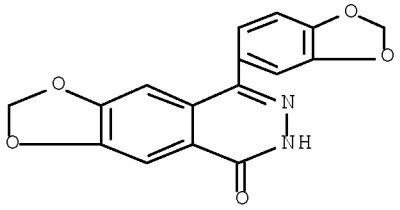
treating or ameliorating the adverse consequences of excitatory amino acid deficiency such as schizophrenia, myoclonus, Alzheimer's disease and malnutrition and neural maldevelopment, and as cognition and learning enhancers.

IT 243134-66-9P

(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

RN 243134-66-9 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)- (CA INDEX NAME)

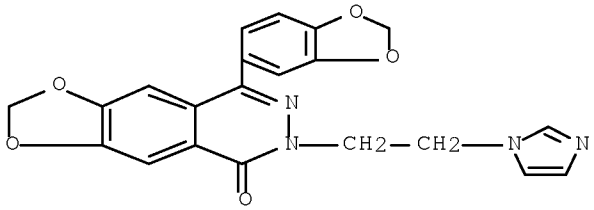


IT 243134-67-0P 243134-68-1P 243134-69-2P 243134-70-5P 243134-71-6P 243134-72-7P

(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

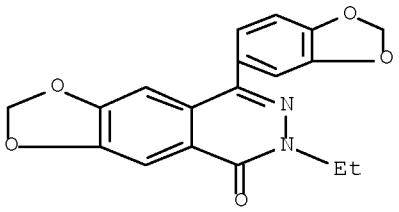
RN 243134-67-0 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)-6-[2-(1H-imidazol-1-yl)ethyl]- (CA INDEX NAME)

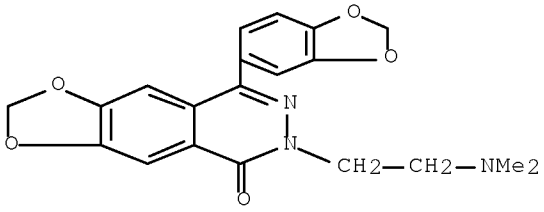


RN 243134-68-1 USPATFULL

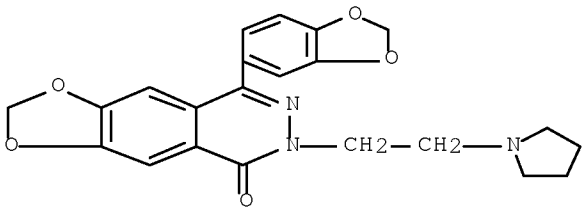
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)-6-ethyl- (CA INDEX NAME)



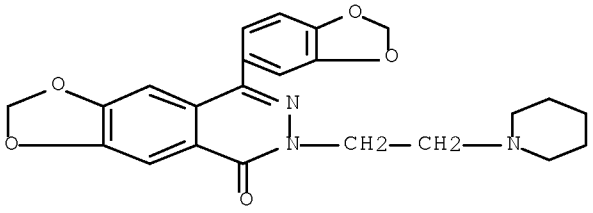
RN 243134-69-2 USPATFULL
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(dimethylamino)ethyl]- (CA INDEX NAME)



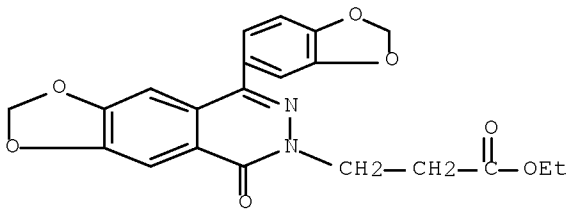
RN 243134-70-5 USPATFULL
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(1-pyrrolidinyl)ethyl]- (CA INDEX NAME)



RN 243134-71-6 USPATFULL
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 243134-72-7 USPATFULL
CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-propanoic acid,
8-(1,3-benzodioxol-5-yl)-5-oxo-, ethyl ester (CA INDEX NAME)



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CONTINUE? (Y)/N:y

L56 ANSWER 10 OF 12 BIOSIS COPYRIGHT (c) 2008 The Thomson Corporation on STN DUPLICATE 1
ACCESSION NUMBER: 2005:473259 BIOSIS Full-text
DOCUMENT NUMBER: PREV200510263078
TITLE: Quinazolinones and benzothiazinones as novel sodium channel blockers.
AUTHOR(S): Victory, Sam F. [Reprint Author]; Sun, Qun; Limberis, Jim; Kyle, Donald J.
CORPORATE SOURCE: Purdue Pharma, Discovery Res, Cranbury, NJ 08512 USA
sam.victory@pharma.com
SOURCE: Abstracts of Papers American Chemical Society, (AUG 22 2004) Vol. 228, No. Part 1, pp. U920.
Meeting Info.: Meeting of the Division of Chemical Toxicology of the American-Chemical-Society held at the 228th National Meeting of the American-Chemical-Society. Philadelphia, PA, USA. August 22 -26, 2004. Amer Chem Soc, Div Chem Toxicol.
CODEN: ACSRAL. ISSN: 0065-7727.
DOCUMENT TYPE: Conference; (Meeting)
Conference; Abstract; (Meeting Abstract)
LANGUAGE: English
ENTRY DATE: Entered STN: 16 Nov 2005
Last Updated on STN: 16 Nov 2005
ED Entered STN: 16 Nov 2005
Last Updated on STN: 16 Nov 2005
CC General biology - Symposia, transactions and proceedings 00520
Biophysics - Membrane phenomena 10508
Pathology - Therapy 12512
Nervous system - Physiology and biochemistry 20504
Nervous system - Pathology 20506
Pharmacology - General 22002
Pharmacology - Neuropharmacology 22024

IT Major Concepts
Pharmacology; Nervous System (Neural Coordination)
IT Diseases
neuropathic pain: nervous system disease, drug therapy
Pain (MeSH)
IT Chemicals & Biochemicals
sodium channel; V102862: analgesic-drug, semicarbazone moiety; sodium channel blockers: analgesic-drug, thiazolidinone ring, hydrophic aryl ether moiety, piperidinylethylamine moiety, quinazolin-4(3H)-one core ring system, 2,3-dyhydro-benzothiazin-4-one core ring system
IT Miscellaneous Descriptors
structure-activity relationship

L56 ANSWER 11 OF 12 BIOSIS COPYRIGHT (c) 2008 The Thomson Corporation on STN
ACCESSION NUMBER: 2004:332648 BIOSIS Full-text
DOCUMENT NUMBER: PREV200400337520
TITLE: Substituted quinazolines and analogs and the use thereof.
AUTHOR(S): Upasani, Ravi [Inventor, Reprint Author]; Cai, Sui X. [Inventor]
CORPORATE SOURCE: Sunnyvale, CA, USA
ASSIGNEE: Euro-Celtique S.A., Luxembourg
PATENT INFORMATION: US 6765006 20040720
SOURCE: Official Gazette of the United States Patent and Trademark Office Patents, (July 20 2004) Vol. 1284, No. 3. http://www.uspto.gov/web/menu/patdata.html. e-file. ISSN: 0098-1133 (ISSN print).
DOCUMENT TYPE: Patent
LANGUAGE: English
ENTRY DATE: Entered STN: 4 Aug 2004
Last Updated on STN: 4 Aug 2004
ED Entered STN: 4 Aug 2004
Last Updated on STN: 4 Aug 2004
AB The invention relates to novel quinazolines and heterocycles which are antagonists or positive modulators of AMPA receptors, and the use thereof for treating, preventing or ameliorating neuronal loss associated with stroke, global and focal ischemia, CNS trauma, hypoglycemia and surgery, as well as treating or ameliorating neurodegenerative diseases including Alzheimer's disease, amyotrophic lateral sclerosis, Huntington's disease, Parkinson's disease and Down's syndrome, treating, preventing or ameliorating the adverse consequences of the overstimulation of the excitatory amino acids, treating, preventing or ameliorating anxiety, psychosis, convulsions, chronic pain, glaucoma, retinitis, urinary incontinence, muscular spasm and inducing anesthesia, as well as for treating or ameliorating the adverse consequences of excitatory amino acid deficiency such as schizophrenia, myoclonus, Alzheimer's disease and malnutrition and neural maldevelopment, and as cognition and learning enhancers.
NCL 514232800
CC Pathology - Therapy 12512
Urinary system - Pathology 15506
Sense organs - Pathology 20006
Nervous system - Pathology 20506
Pharmacology - General 22002
Pharmacology - Neuropharmacology 22024
Pharmacology - Psychopharmacology 22026
Pharmacology - Sense organs, associated structures and functions 22031
IT Major Concepts

```
        Pharmacology
IT   Diseases
        anxiety: behavioral and mental disorders, drug therapy
        Anxiety (MeSH)
IT   Diseases
        glaucoma: eye disease, drug therapy
        Glaucoma (MeSH)
IT   Diseases
        malnutrition: nutritional disease, drug therapy
        Nutrition Disorders (MeSH)
IT   Diseases
        neurological diseases: nervous system disease, drug therapy
IT   Diseases
        psychosis: behavioral and mental disorders, drug therapy
        Psychotic Disorders (MeSH)
IT   Diseases
        retinitis: eye disease, drug therapy
        Retinitis (MeSH)
IT   Diseases
        schizophrenia: behavioral and mental disorders, drug therapy
        Schizophrenia (MeSH)
IT   Diseases
        urinary incontinence: urologic disease, drug therapy
        Urinary Incontinence (MeSH)
IT   Chemicals & Biochemicals
        substituted quinazolines: anticonvulsant-drug,
        antiglaucoma-drug, antiparkinsonian-drug, antipsychotic-drug, general
        anesthetic-drug, neuroprotectant-drug, nootropic-drug, ophthalmic-drug,
        AMPA receptor antagonists, analogs
RN   253-82-7D (substituted quinazolines)

L56  ANSWER 12 OF 12  SCISEARCH  COPYRIGHT (c) 2008 The Thomson Corporation  on
     STN
ACCESSION NUMBER:    2004:180442  SCISEARCH  Full-text
THE GENUINE ARTICLE: 751JG
TITLE:               Facile thermal conversion of arylcyanoguanidines to 2,4-
                     diaminoquinazolines.
AUTHOR:              Shao B (Reprint); Huang J C
CORPORATE SOURCE:    Purdue Pharma, Computat Combinatorial
                     & Med Chem Dept, LP, Cranbury, NJ 08512 USA
COUNTRY OF AUTHOR:   USA
SOURCE:              ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, (SEP
                     2003) Vol. 226, Part 2, pp. U180-U180. MA 401-ORGN.
                     ISSN: 0065-7727.
PUBLISHER:           AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036
                     USA.
DOCUMENT TYPE:       Conference; Journal
LANGUAGE:            English
REFERENCE COUNT:     0
ENTRY DATE:          Entered STN: 5 Mar 2004
                     Last Updated on STN: 5 Mar 2004
ED   Entered STN: 5 Mar 2004
     Last Updated on STN: 5 Mar 2004
CC   CHEMISTRY, MULTIDISCIPLINARY


=> file stnguide
FILE 'STNGUIDE' ENTERED AT 16:01:23 ON 04 DEC 2008
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov 21, 2008 (20081121/UP).

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     FILE 'HCAPLUS' ENTERED AT 13:48:53 ON 04 DEC 2008
L1             1 SEA SPE=ON  ABB=ON  PLU=ON  US2004-772445/APPS

     FILE 'WPIX' ENTERED AT 13:49:03 ON 04 DEC 2008
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     FILE 'STNGUIDE' ENTERED AT 13:49:16 ON 04 DEC 2008
                D QUE L1

     FILE 'HCAPLUS' ENTERED AT 13:49:41 ON 04 DEC 2008
                D IBIB ED ABS IND L1

     FILE 'STNGUIDE' ENTERED AT 13:49:48 ON 04 DEC 2008
                D QUE L2

     FILE 'WPIX' ENTERED AT 13:50:15 ON 04 DEC 2008
                D IALL CODE L2

     FILE 'STNGUIDE' ENTERED AT 13:50:16 ON 04 DEC 2008

     FILE 'REGISTRY' ENTERED AT 13:50:28 ON 04 DEC 2008

     FILE 'HCAPLUS' ENTERED AT 13:50:31 ON 04 DEC 2008
L3             TRA PLU=ON  L1 1- RN :     213 TERMS

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L4           213 SEA SPE=ON  ABB=ON  PLU=ON  L3
L5             7 SEA SPE=ON  ABB=ON  PLU=ON  L4 AND N2C4/ESS
                D SCAN

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L6             STR

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L7             0 SEA SSS SAM L6
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     FILE 'LREGISTRY' ENTERED AT 13:55:08 ON 04 DEC 2008
L*** DEL        STR L6
L8             STR L***

     FILE 'REGISTRY' ENTERED AT 13:56:40 ON 04 DEC 2008
L9             0 SEA SSS SAM L8

     FILE 'STNGUIDE' ENTERED AT 13:56:47 ON 04 DEC 2008
                D QUE STAT

     FILE 'REGISTRY' ENTERED AT 14:04:48 ON 04 DEC 2008
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                D SCAN L5
L10           56 SEA SSS FUL L8
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                D SCAN

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L11             STR L8

     FILE 'REGISTRY' ENTERED AT 14:14:16 ON 04 DEC 2008
L12            2 SEA SUB=L10 SSS SAM L11
                D SCAN

     FILE 'STNGUIDE' ENTERED AT 14:14:29 ON 04 DEC 2008
                D QUE STAT

     FILE 'LREGISTRY' ENTERED AT 14:17:36 ON 04 DEC 2008
L13             STR L11

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L14            2 SEA SUB=L10 SSS SAM L13

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     FILE 'REGISTRY' ENTERED AT 14:24:50 ON 04 DEC 2008
                D QUE STAT
L15           37 SEA SUB=L10 SSS FUL L13
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L16           17 SEA SPE=ON  ABB=ON  PLU=ON  L15

     FILE 'STNGUIDE' ENTERED AT 14:28:10 ON 04 DEC 2008

     FILE 'REGISTRY' ENTERED AT 14:28:58 ON 04 DEC 2008
L17             ANALYZE PLU=ON  L15 1- LC :       8 TERMS
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     FILE 'STNGUIDE' ENTERED AT 14:30:20 ON 04 DEC 2008

     FILE 'REGISTRY' ENTERED AT 14:31:25 ON 04 DEC 2008
L18            0 SEA SPE=ON  ABB=ON  PLU=ON  L5 NOT L15

     FILE 'STNGUIDE' ENTERED AT 14:31:41 ON 04 DEC 2008

     FILE 'STNGUIDE' ENTERED AT 15:27:05 ON 04 DEC 2008

     FILE 'ZCAPLUS' ENTERED AT 15:27:13 ON 04 DEC 2008
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L20             QUE SPE=ON  ABB=ON  PLU=ON  CAI, S?/AU
L21             QUE SPE=ON  ABB=ON  PLU=ON  LAN, N?/AU
L22             QUE SPE=ON  ABB=ON  PLU=ON  WANG, Y?/AU
L23             QUE SPE=ON  ABB=ON  PLU=ON  FIELD, G?/AU
L24             QUE SPE=ON  ABB=ON  PLU=ON  FICK, D?/AU
L25             QUE SPE=ON  ABB=ON  PLU=ON  (COCENSYS OR (PURDUE(1W)PHARMA) OR
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L26             QUE SPE=ON  ABB=ON  PLU=ON  AY<2000 OR PY<2000 OR PRY<2000 OR
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L27           17 SEA SPE=ON  ABB=ON  PLU=ON  L15

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     FILE 'HCAPLUS' ENTERED AT 15:30:58 ON 04 DEC 2008
L28            1 SEA SPE=ON  ABB=ON  PLU=ON  L27 AND (L19 OR L20 OR L21 OR L22
                 OR L23 OR L24 OR L25)
L29            1 SEA SPE=ON  ABB=ON  PLU=ON  L1 AND L28
L30            1 SEA SPE=ON  ABB=ON  PLU=ON  (L28 OR L29)
L31           16 SEA SPE=ON  ABB=ON  PLU=ON  L27 NOT L30

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L32            9 SEA SPE=ON  ABB=ON  PLU=ON  L15
L33            3 SEA SPE=ON  ABB=ON  PLU=ON  L32 AND (L19 OR L20 OR L21 OR L22
                 OR L23 OR L24 OR L25)
L34            6 SEA SPE=ON  ABB=ON  PLU=ON  L32 NOT L33

     FILE 'STNGUIDE' ENTERED AT 15:32:46 ON 04 DEC 2008

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L35            1 SEA SPE=ON  ABB=ON  PLU=ON  L15
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L36            2 SEA SPE=ON  ABB=ON  PLU=ON  CA52:15486I/OREF

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L37            3 SEA SPE=ON  ABB=ON  PLU=ON  L15

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     FILE 'BEILSTEIN' ENTERED AT 15:34:14 ON 04 DEC 2008
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L38            0 SEA SSS SAM L13
                 D QUE STAT
L39           33 SEA SSS FUL L13

     FILE 'CHEMINFORMRX' ENTERED AT 15:35:19 ON 04 DEC 2008
L40            0 SEA SSS SAM L13 (     0 REACTIONS)
L41            4 SEA SSS FUL L13 (     8 REACTIONS)
L42            0 SEA SPE=ON  ABB=ON  PLU=ON  L41 AND (L19 OR L20 OR L21 OR L22
                 OR L23 OR L24 OR L25)
L43            4 SEA SPE=ON  ABB=ON  PLU=ON  L41 NOT L42

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L44            0 SEA SSS SAM L13
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L45            8 SEA SSS FUL L13
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                 SELECT L45 1- SDCN
L46            1 SEA SPE=ON  ABB=ON  PLU=ON  (RA0ON1/DCN OR RA0ON2/DCN OR
                 RA0ON3/DCN OR RA0ON4/DCN OR RA0ON5/DCN OR RA0ON6/DCN OR
                 RA0ON7/DCN OR RA0ON8/DCN) OR L45/DCR
L47            1 SEA SPE=ON  ABB=ON  PLU=ON  L46 AND (L19 OR L20 OR L21 OR L22
                 OR L23 OR L24 OR L25)
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L48           1 SEA SPE=ON  ABB=ON  PLU=ON  L47 OR L2
L49           1 SEA SPE=ON  ABB=ON  PLU=ON  L47 AND L2
L50           1 SEA SPE=ON  ABB=ON  PLU=ON  L47 OR L49
L51           0 SEA SPE=ON  ABB=ON  PLU=ON  L46 NOT L50

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L52         164 SEA SPE=ON  ABB=ON  PLU=ON  (L19 OR L20 OR L21 OR L22 OR L23
                OR L24 OR L25) AND ?QUINAZOLIN?/IT,TI,CC,CT,ST,STP
                D QUE
L53          37 SEA SPE=ON  ABB=ON  PLU=ON  L52 AND (L19 OR L23 OR L21 OR L24)

L54          15 SEA SPE=ON  ABB=ON  PLU=ON  L52 AND L25

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                D QUE STAT L15
                D QUE NOS L17
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                D QUE NOS L31
                D QUE NOS L34
                D QUE NOS L35
                D QUE NOS L36
                D QUE NOS L37
                D QUE STAT L41
                D QUE NOS L43
                D QUE STAT L45
                D QUE NOS L51

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L55          24 DUP REM L31 L34 L35 L36 L37 L43 L51 (8 DUPLICATES REMOVED)
                     ANSWERS '1-16' FROM FILE HCAPLUS
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                     ANSWERS '18-20' FROM FILE CHEMCATS
                     ANSWERS '21-24' FROM FILE CHEMINFORMRX
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     FILE 'HCAPLUS, CAOLD, CHEMCATS, CHEMINFORMRX' ENTERED AT 15:49:10 ON 04
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     FILE 'STNGUIDE' ENTERED AT 15:49:10 ON 04 DEC 2008

     FILE 'HCAPLUS, CAOLD, CHEMCATS, CHEMINFORMRX' ENTERED AT 15:49:21 ON 04
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FILE 'HCAPLUS, CAOLD, CHEMCATS, CHEMINFORMRX' ENTERED AT 15:49:47 ON 04
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FILE 'STNGUIDE' ENTERED AT 15:49:48 ON 04 DEC 2008

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                D QUE NOS L42
                D QUE L45
                D QUE NOS L50
                D QUE L54

     FILE 'HCAPLUS, USPATFULL, WPIX, BIOSIS, EMBASE, DRUGU, SCISEARCH' ENTERED
     AT 15:58:57 ON 04 DEC 2008
L56           12 DUP REM L30 L33 L42 L50 L54 (8 DUPLICATES REMOVED)
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                     ANSWERS '7-9' FROM FILE USPATFULL
                     ANSWERS '10-11' FROM FILE BIOSIS
                     ANSWER '12' FROM FILE SCISEARCH
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     FILE 'STNGUIDE' ENTERED AT 15:59:14 ON 04 DEC 2008

     FILE 'HCAPLUS, USPATFULL, BIOSIS, SCISEARCH' ENTERED AT 15:59:34 ON 04
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                D IBIB ED ABS HITIND HITSTR 1-6

     FILE 'STNGUIDE' ENTERED AT 15:59:36 ON 04 DEC 2008

     FILE 'HCAPLUS, USPATFULL, BIOSIS, SCISEARCH' ENTERED AT 16:00:01 ON 04
     DEC 2008
                D IBIB AB HITSTR 7-9

     FILE 'STNGUIDE' ENTERED AT 16:00:10 ON 04 DEC 2008

     FILE 'HCAPLUS, USPATFULL, BIOSIS, SCISEARCH' ENTERED AT 16:00:25 ON 04
     DEC 2008
                D IBIB ED AB IND 10-12

     FILE 'STNGUIDE' ENTERED AT 16:00:25 ON 04 DEC 2008

     FILE 'STNGUIDE' ENTERED AT 16:01:23 ON 04 DEC 2008


     FILE HOME

     FILE STNGUIDE
     FILE CONTAINS CURRENT INFORMATION.
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LAST RELOADED: Nov 21, 2008 (20081121/UP).

FILE ZCAPLUS

FILE COVERS 1907 - 4 Dec 2008 VOL 149 ISS 23
FILE LAST UPDATED: 3 Dec 2008 (20081203/ED)

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE HCAPLUS

FILE COVERS 1907 - 4 Dec 2008 VOL 149 ISS 23
FILE LAST UPDATED: 3 Dec 2008 (20081203/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE WPIX
FILE LAST UPDATED: 28 NOV 2008 <20081128/UP>
MOST RECENT UPDATE: 200877 <200877/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE
>>> Now containing more than 1.2 million chemical structures in DCR <<<

>>> IPC Reform backfile reclassifications have been loaded to end of September 2008. No update date (UP) has been created for the reclassified documents, but they can be identified by 20060101/UPIC, and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC, 20071130/UPIC, 20080401/UPIC, 20080701/UPIC and 20081001/UPIC.
ECLA reclassifications to mid August and US national classification

mid September 2008 have also been loaded. Update dates 20080401, 20080701 and 20081001/UPEC and /UPNC have been assigned to these. <<

FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE, PLEASE VISIT:
http://www.stn-international.de/training_center/patents/stn_guide.pdf

FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE
http://scientific.thomsonreuters.com/support/patents/coverage/latestupdate

EXPLORE DERWENT WORLD PATENTS INDEX IN STN ANAVIST, VERSION 2.0:
http://www.stn-international.com/DWPIAnaVist2_0608.html

>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

FILE REGISTRY
Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 DEC 2008 HIGHEST RN 1078799-92-4
DICTIONARY FILE UPDATES: 2 DEC 2008 HIGHEST RN 1078799-92-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

FILE LREGISTRY
LREGISTRY IS A STATIC LEARNING FILE

NEW CAS INFORMATION USE POLICIES, ENTER HELP USAGETERMS FOR DETAILS.

FILE USPATFULL
FILE COVERS 1971 TO PATENT PUBLICATION DATE: 4 Dec 2008 (20081204/PD)
FILE LAST UPDATED: 4 Dec 2008 (20081204/ED)
HIGHEST GRANTED PATENT NUMBER: US7461407
HIGHEST APPLICATION PUBLICATION NUMBER: US20080301844
CA INDEXING IS CURRENT THROUGH 4 Dec 2008 (20081204/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 4 Dec 2008 (20081204/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2008
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2008

USPATFULL now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

FILE USPATOLD

FILE COVERS U.S. PATENTS 1790-1975
Produced using data provided by Univentio.

This database was created using Optical Character Recognition (OCR) technology. For this reason, some characters may be missing or mistranslated. In order to improve searchability and retrieval, CA indexing information has been added to the Title, Inventor, and Patent Assignee fields where possible. Please see HELP CASDATA for more information on the availability of CAS indexing in this database.

USPATOLD now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

FILE USPAT2

FILE COVERS 2001 TO PUBLICATION DATE: 4 Dec 2008 (20081204/PD)
FILE LAST UPDATED: 4 Dec 2008 (20081204/ED)
HIGHEST GRANTED PATENT NUMBER: US20080227788
HIGHEST APPLICATION PUBLICATION NUMBER: US20080300718
CA INDEXING IS CURRENT THROUGH 4 Dec 2008 (20081204/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 4 Dec 2008 (20081204/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2008
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2008

USPAT2 now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

FILE CASREACT

FILE CONTENT:1840 - 29 Nov 2008 VOL 149 ISS 23

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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**********************************************************
*                                                        *
*     CASREACT now has more than 15.3 million reactions  *
*                                                        *
**********************************************************
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CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE TOXCENTER

FILE COVERS 1907 TO 2 Dec 2008 (20081202/ED)

The MEDLINE file segment has been updated with the National Library of Medicine's revised 2008 MeSH terms. See HELP RLOAD for details.

This file contains CAS Registry Numbers for easy and accurate substance

identification.

The BIOSIS segment of TOXCENTER has been augmented with 13,000 records from 1946 through 1968.

FILE CAOLD
FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

CAOLD will be discontinued and removed from associated database clusters.

. November 22, 2008 - removed from database clusters
. December 31, 2008 - removed from STN

Content previously available only in CAOLD is now available in CA/CAplus. To learn more about the options available for transferring saved search queries and answer sets to CA/CAplus, contact your STN Service Center.

FILE CHEMCATS

FILE LAST UPDATED 22 NOVEMBER 2008 (20081122/UP)

For details on recent updates in CHEMCATS, enter NEWS FILE at an arrow prompt. For the list of suppliers currently in the file, enter HELP SPA, HELP SPB, HELP SPC, HELP SPDH, HELP SPIN, HELP SPOQ, HELP SPRS, and HELP SPTZ. For the list of current catalogs, enter HELP CTA, HELP CTB, HELP CTC, HELP CTDH, HELP CTIL, HELP CTMN, HELP CTOQ, HELP CTRS, and HELP CTTZ.

This database is provided on an "as is" basis. Please consult the suppliers for current information regarding pricing, regional availability, available quantities, purities, etc. THERE ARE NO WARRANTIES OF ANY KIND, EITHER EXPRESSED OR IMPLIED. ACS is not liable for any loss of profit, goodwill or any other damages arising out of the use of this database.

CHEMCATS now contains more than 25 million records. See HELP CONTENT and NEWS FILE for details.

FILE BEILSTEIN
FILE LAST UPDATED ON April 1, 2008

FILE COVERS 1771 TO 2008.
FILE CONTAINS 10,322,808 SUBSTANCES

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>>>PLEASE NOTE: Reaction Data and substance data are stored in
   separate documents and can not be searched together in one query.
   Reaction data for BEILSTEIN compounds may be displayed
   immediately with the display codes PRE (preparations) and REA
   (reactions).  A substance answer set retrieved after the search
   for a chemical name, a compounds with available reaction
   information by combining with PRE/FA, REA/FA or more generally
   with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
   between a BEILSTEIN compound and belonging reactions. For mo
   detailed reaction searches BRNs can be searched as reaction
   partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE  <<<

**********************************************************************
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.                 *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE    *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE           *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                         *
* FOR PRICE INFORMATION SEE HELP COST                                 *
**********************************************************************

>>> Price change as of January 1st, 2008: Connect Time and Structure
    Search fees re-introduced. See NEWS and HELP COST <<<

FILE CHEMINFORMRX
FILE LAST UPDATED: 16 OCT 2008       <20081016/UP>

>>> CAS Registry Numbers are available for
    substances prior to 1995   <<<

FILE MEDLINE
 FILE LAST UPDATED: 3 Dec 2008 (20081203/UP).  FILE COVERS 1949 TO DATE.

  MEDLINE has been updated with the National Library of Medicine's
  revised 2008 MeSH terms.  See HELP RLOAD for details.

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.

  See HELP RANGE before carrying out any RANGE search.

  MEDLINE Accession Numbers (ANs) for records from 1950-1977 have
  been converted from 8 to 10 digits.  Searches using an 8 or 10 digit
  AN will retrieve the same record.  The 10-digit ANs can be expanded,
  searched, and displayed in all records from 1949 to the present.

FILE BIOSIS
FILE COVERS 1926 TO DATE.
CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT
FROM JANUARY 1926 TO DATE.

RECORDS LAST ADDED: 3 December 2008 (20081203/ED)

BIOSIS has been augmented with 1.8 million archival records from 1926
through 1968.  These records have been re-indexed to match current
BIOSIS indexing.

FILE EMBASE
 FILE COVERS 1974 TO 3 Dec 2008 (20081203/ED)
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EMBASE was reloaded on March 30, 2008.

EMBASE is now updated daily. SDI frequency remains weekly (default) and biweekly.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Beginning January 2008, Elsevier will no longer provide EMTREE codes as part of the EMTREE thesaurus in EMBASE. Please update your current-awareness alerts (SDIs) if they contain EMTREE codes.

For further assistance, please contact your local helpdesk.

FILE PASCAL
FILE LAST UPDATED: 1 DEC 2008 <20081201/UP>
FILE COVERS 1977 TO DATE.

>>> SIMULTANEOUS LEFT AND RIGHT TRUNCATION IS AVAILABLE IN THE BASIC INDEX (/BI) FIELD <<<

FILE CABA
FILE COVERS 1973 TO 6 Nov 2008 (20081106/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

The CABA file was reloaded 7 December 2003. Enter HELP RLOAD for details.

FILE CEABA-VTB
FILE LAST UPDATED: 17 NOV 2008 <20081117/UP>
FILE COVERS 1966 TO DATE

>>> DECHEMA, the producer of CEABA-VTB is using a new classification scheme.
The new classification schemes are available as a PDF file and may be downloaded free-of-charge from:
http://www.stn-international.de/news/cc-de.pdf
and
http://www.stn-international.de/news/cc-en.pdf <<<

FILE LIFESCI
FILE COVERS 1978 TO 13 Nov 2008 (20081113/ED)

FILE BIOENG
FILE LAST UPDATED: 27 OCT 2008 <20081027/UP>
FILE COVERS 1982 TO DATE

>>> SIMULTANEOUS LEFT AND RIGHT TRUNCATION AVAILABLE IN THE BASIC INDEX <<<

FILE BIOTECHNO
FILE LAST UPDATED: 7 JAN 2004 <20040107/UP>
FILE COVERS 1980 TO 2003.
THIS FILE IS A STATIC FILE WITH NO UPDATES

>>> SIMULTANEOUS LEFT AND RIGHT TRUNCATION AVAILABLE IN /CT AND BASIC INDEX <<<

FILE BIOTECHDS
FILE LAST UPDATED: 1 DEC 2008 <20081201/UP>
FILE COVERS 1982 TO DATE

>>> USE OF THIS FILE IS LIMITED TO BIOTECH SUBSCRIBERS <<<

FILE DRUGU
FILE LAST UPDATED: 1 DEC 2008 <20081201/UP>
>>> DERWENT DRUG FILE (SUBSCRIBER) <<<

>>> FILE COVERS 1983 TO DATE <<<
>>> THESAURUS AVAILABLE IN /CT <<<

FILE DRUGB
>>> FILE COVERS 1964 TO 1982 - CLOSED FILE <<<

FILE VETU
FILE LAST UPDATED: 2 JAN 2002 <20020102/UP>
FILE COVERS 1983-2001

FILE VETB
FILE LAST UPDATED: 25 SEP 94 <940925/UP>
FILE COVERS 1968-1982

FILE SCISEARCH

FILE COVERS 1974 TO 27 Nov 2008 (20081127/ED)

SCISEARCH has been reloaded, see HELP RLOAD for details.

FILE CONFSCI
FILE COVERS 1973 TO 6 Nov 2008 (20081106/ED)

CSA has resumed updates, see NEWS FILE

FILE DISSABS
FILE COVERS 1861 TO 24 OCT 2008 (20081024/ED)

FILE RDISCLOSURE
FILE LAST UPDATED: 12 NOV 2008 <20081112/UP>
FILE COVERS 1960 TO DATE

>>> SIMULTANEOUS LEFT AND RIGHT TRUNCATION IS AVAILABLE IN THE BASIC INDEX (/BI) AND TITLE (/TI) FIELDS <<<

>>> IMAGES ARE AVAILABLE ONLINE AND FOR EMAIL-PRINTS <<<

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